



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:50 PM UTC

PDB ID : 3KOX / pdb_00003kox
Title : Crystal Structure of ornithine 4,5 aminomutase in complex with 2,4-diaminobutyrate (Anaerobic)
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on : 2009-11-14
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

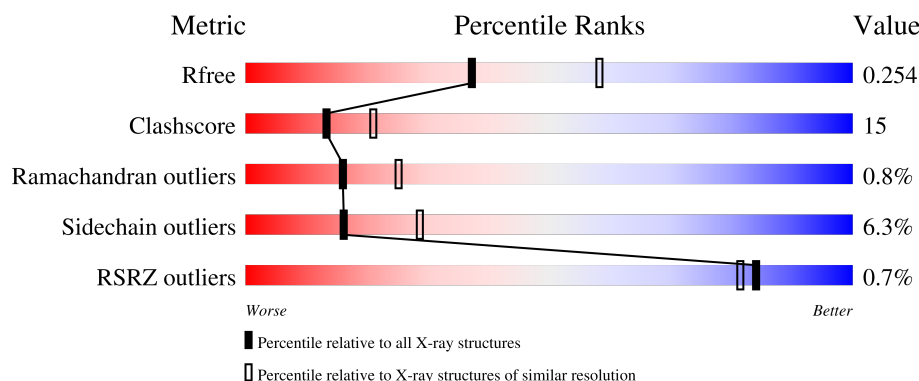
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	763	2% 70% 23% • 5%
1	B	763	71% 22% • 5%
1	C	763	68% 24% • 5%
1	D	763	71% 21% • 5%
2	E	121	69% 19% • 10%

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Mol	Chain	Length	Quality of chain
2	F	121	 % 64% 26% 10%
2	G	121	 % 66% 22% 10%
2	H	121	 % 74% 15% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	A	1801	X	-	-	-
3	B12	B	1801	X	-	-	-
3	B12	C	1801	X	-	-	-
4	5AD	A	1500	X	-	-	-
4	5AD	D	1500	X	-	-	-
5	Z98	A	767	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5651	3561	981	1075	34			
1	B	728	Total	C	N	O	S	0	0	0
			5672	3579	984	1075	34			
1	C	728	Total	C	N	O	S	0	0	0
			5654	3570	981	1069	34			
1	D	728	Total	C	N	O	S	0	0	0
			5664	3575	984	1071	34			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
A	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
A	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
A	744	SER	-	expression tag	UNP Q8VPJ5
A	745	GLU	-	expression tag	UNP Q8VPJ5
A	746	ASP	-	expression tag	UNP Q8VPJ5
A	747	PRO	-	expression tag	UNP Q8VPJ5
A	748	ASN	-	expression tag	UNP Q8VPJ5
A	749	SER	-	expression tag	UNP Q8VPJ5
A	750	SER	-	expression tag	UNP Q8VPJ5
A	751	SER	-	expression tag	UNP Q8VPJ5
A	752	VAL	-	expression tag	UNP Q8VPJ5
A	753	ASP	-	expression tag	UNP Q8VPJ5
A	754	LYS	-	expression tag	UNP Q8VPJ5
A	755	LEU	-	expression tag	UNP Q8VPJ5
A	756	ALA	-	expression tag	UNP Q8VPJ5
A	757	ALA	-	expression tag	UNP Q8VPJ5
A	758	ALA	-	expression tag	UNP Q8VPJ5
A	759	LEU	-	expression tag	UNP Q8VPJ5
A	760	GLU	-	expression tag	UNP Q8VPJ5
A	761	HIS	-	expression tag	UNP Q8VPJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	762	HIS	-	expression tag	UNP Q8VPJ5
A	763	HIS	-	expression tag	UNP Q8VPJ5
A	764	HIS	-	expression tag	UNP Q8VPJ5
A	765	HIS	-	expression tag	UNP Q8VPJ5
A	766	HIS	-	expression tag	UNP Q8VPJ5
B	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
B	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
B	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
B	744	SER	-	expression tag	UNP Q8VPJ5
B	745	GLU	-	expression tag	UNP Q8VPJ5
B	746	ASP	-	expression tag	UNP Q8VPJ5
B	747	PRO	-	expression tag	UNP Q8VPJ5
B	748	ASN	-	expression tag	UNP Q8VPJ5
B	749	SER	-	expression tag	UNP Q8VPJ5
B	750	SER	-	expression tag	UNP Q8VPJ5
B	751	SER	-	expression tag	UNP Q8VPJ5
B	752	VAL	-	expression tag	UNP Q8VPJ5
B	753	ASP	-	expression tag	UNP Q8VPJ5
B	754	LYS	-	expression tag	UNP Q8VPJ5
B	755	LEU	-	expression tag	UNP Q8VPJ5
B	756	ALA	-	expression tag	UNP Q8VPJ5
B	757	ALA	-	expression tag	UNP Q8VPJ5
B	758	ALA	-	expression tag	UNP Q8VPJ5
B	759	LEU	-	expression tag	UNP Q8VPJ5
B	760	GLU	-	expression tag	UNP Q8VPJ5
B	761	HIS	-	expression tag	UNP Q8VPJ5
B	762	HIS	-	expression tag	UNP Q8VPJ5
B	763	HIS	-	expression tag	UNP Q8VPJ5
B	764	HIS	-	expression tag	UNP Q8VPJ5
B	765	HIS	-	expression tag	UNP Q8VPJ5
B	766	HIS	-	expression tag	UNP Q8VPJ5
C	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
C	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
C	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
C	744	SER	-	expression tag	UNP Q8VPJ5
C	745	GLU	-	expression tag	UNP Q8VPJ5
C	746	ASP	-	expression tag	UNP Q8VPJ5
C	747	PRO	-	expression tag	UNP Q8VPJ5
C	748	ASN	-	expression tag	UNP Q8VPJ5
C	749	SER	-	expression tag	UNP Q8VPJ5
C	750	SER	-	expression tag	UNP Q8VPJ5
C	751	SER	-	expression tag	UNP Q8VPJ5

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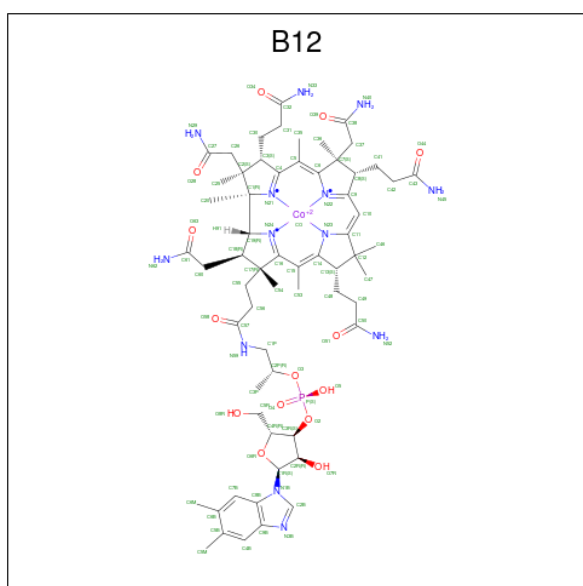
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	expression tag	UNP Q8VPJ5
C	758	ALA	-	expression tag	UNP Q8VPJ5
C	759	LEU	-	expression tag	UNP Q8VPJ5
C	760	GLU	-	expression tag	UNP Q8VPJ5
C	761	HIS	-	expression tag	UNP Q8VPJ5
C	762	HIS	-	expression tag	UNP Q8VPJ5
C	763	HIS	-	expression tag	UNP Q8VPJ5
C	764	HIS	-	expression tag	UNP Q8VPJ5
C	765	HIS	-	expression tag	UNP Q8VPJ5
C	766	HIS	-	expression tag	UNP Q8VPJ5
D	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
D	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
D	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
D	744	SER	-	expression tag	UNP Q8VPJ5
D	745	GLU	-	expression tag	UNP Q8VPJ5
D	746	ASP	-	expression tag	UNP Q8VPJ5
D	747	PRO	-	expression tag	UNP Q8VPJ5
D	748	ASN	-	expression tag	UNP Q8VPJ5
D	749	SER	-	expression tag	UNP Q8VPJ5
D	750	SER	-	expression tag	UNP Q8VPJ5
D	751	SER	-	expression tag	UNP Q8VPJ5
D	752	VAL	-	expression tag	UNP Q8VPJ5
D	753	ASP	-	expression tag	UNP Q8VPJ5
D	754	LYS	-	expression tag	UNP Q8VPJ5
D	755	LEU	-	expression tag	UNP Q8VPJ5
D	756	ALA	-	expression tag	UNP Q8VPJ5
D	757	ALA	-	expression tag	UNP Q8VPJ5
D	758	ALA	-	expression tag	UNP Q8VPJ5
D	759	LEU	-	expression tag	UNP Q8VPJ5
D	760	GLU	-	expression tag	UNP Q8VPJ5
D	761	HIS	-	expression tag	UNP Q8VPJ5
D	762	HIS	-	expression tag	UNP Q8VPJ5
D	763	HIS	-	expression tag	UNP Q8VPJ5
D	764	HIS	-	expression tag	UNP Q8VPJ5
D	765	HIS	-	expression tag	UNP Q8VPJ5
D	766	HIS	-	expression tag	UNP Q8VPJ5

- Molecule 2 is a protein called D-ornithine aminomutase S component.

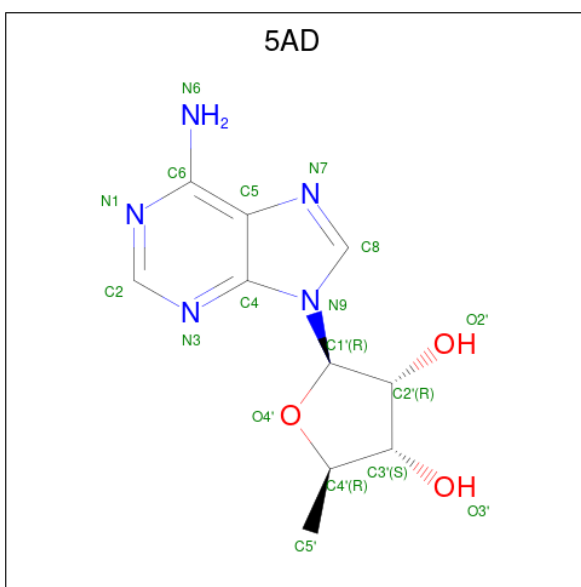
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	F	109	Total	C	N	O	S	0	0	0
			858	539	152	163	4			
2	G	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	H	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



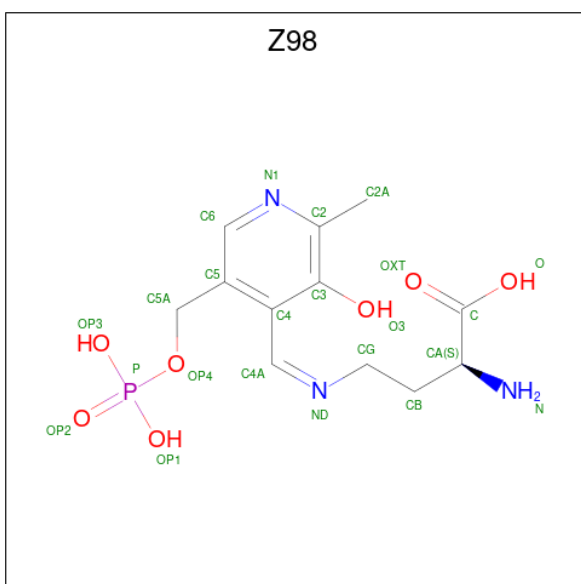
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 4 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	10	5	3		
4	B	1	Total	C	N	O	0	0
			18	10	5	3		
4	C	1	Total	C	N	O	0	0
			18	10	5	3		
4	D	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 5 is (2S)-2-amino-4-[(1Z)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}butanoic acid (CCD ID: Z98) (formula: C₁₂H₁₈N₃O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 23	C 12	N 3	O 7	P 1	0	0
5	B	1	Total 23	C 12	N 3	O 7	P 1	0	0
5	C	1	Total 23	C 12	N 3	O 7	P 1	0	0
5	D	1	Total 23	C 12	N 3	O 7	P 1	0	0

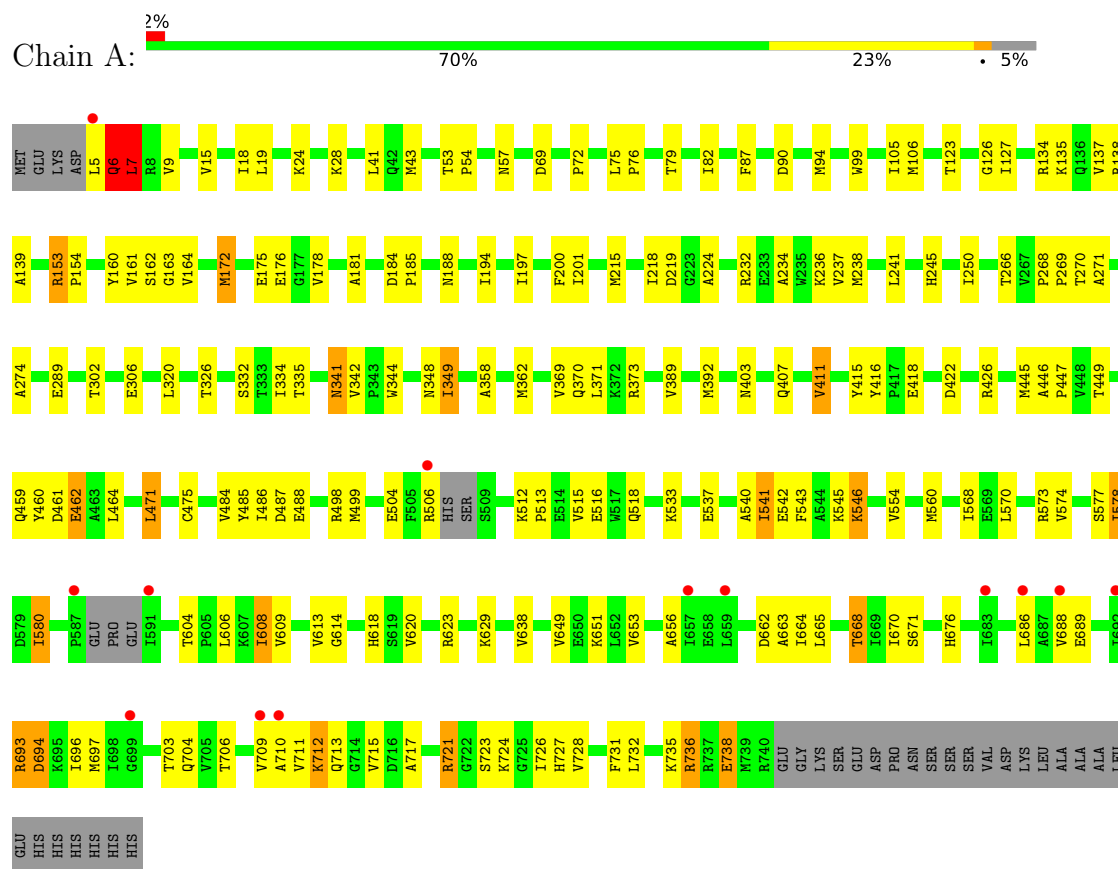
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total 144	O 144	0	0
6	E	15	Total 15	O 15	0	0
6	B	199	Total 199	O 199	0	0
6	F	33	Total 33	O 33	0	0
6	C	145	Total 145	O 145	0	0
6	G	17	Total 17	O 17	0	0
6	D	217	Total 217	O 217	0	0
6	H	17	Total 17	O 17	0	0

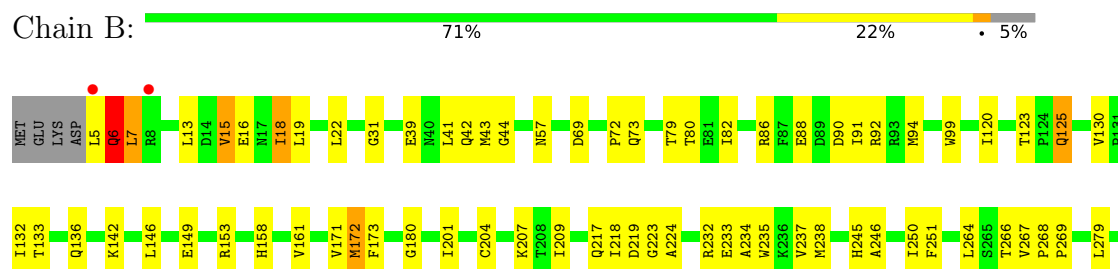
3 Residue-property plots [i](#)

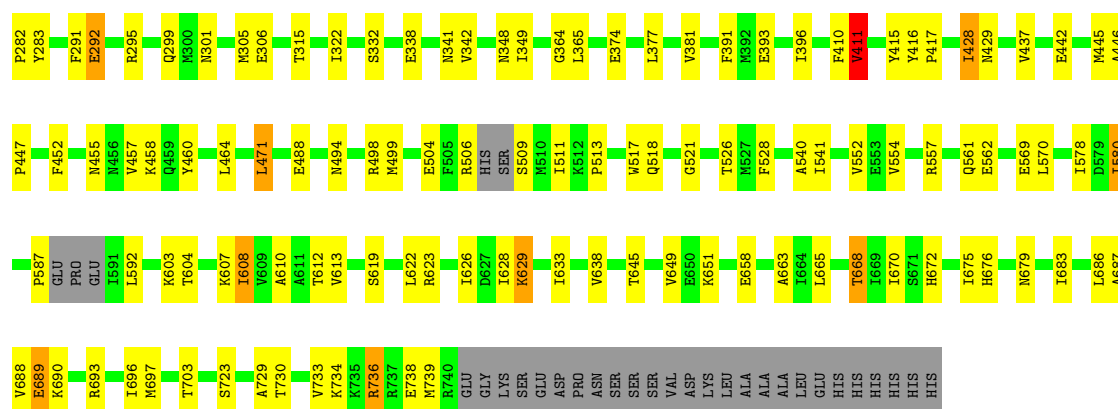
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: D-ornithine aminomutase E component



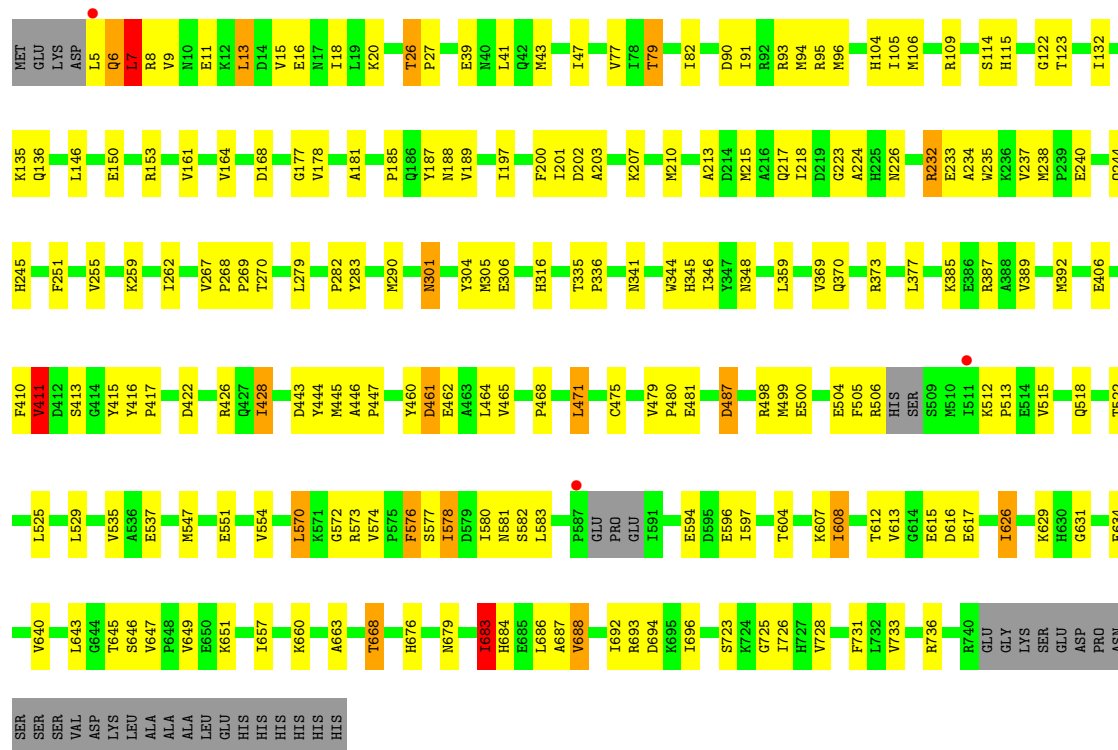
- Molecule 1: D-ornithine aminomutase E component





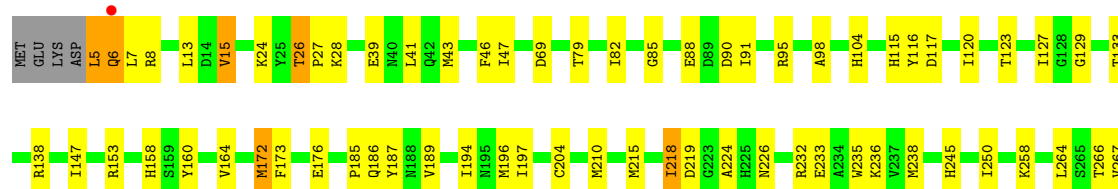
• Molecule 1: D-ornithine aminomutase E component

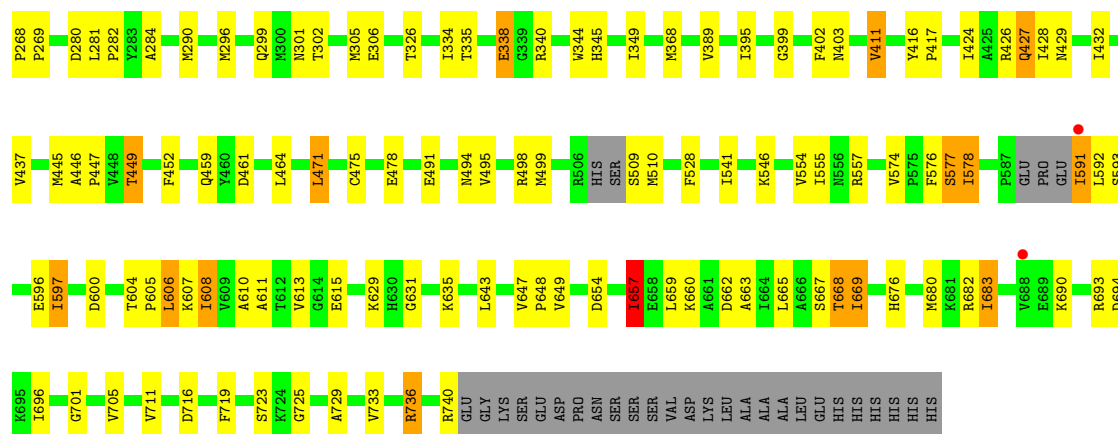
Chain C: 68% 24% 5%



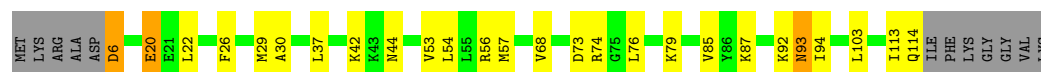
• Molecule 1: D-ornithine aminomutase E component

Chain D: 71% 21% 5%





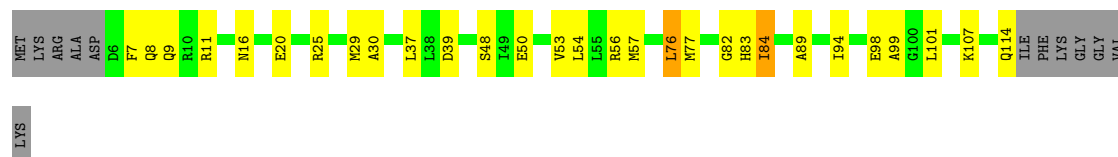
• Molecule 2: D-ornithine aminomutase S component



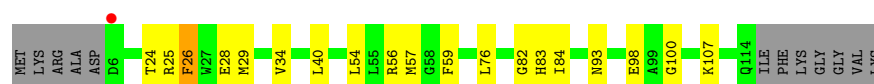
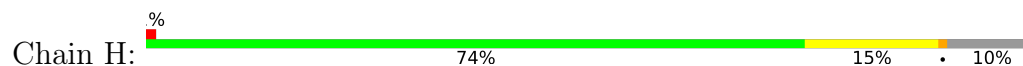
• Molecule 2: D-ornithine aminomutase S component



• Molecule 2: D-ornithine aminomutase S component



• Molecule 2: D-ornithine aminomutase S component



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.96Å 231.69Å 123.89Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	64.23 – 2.40 64.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.23-2.40) 99.9 (64.23-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.190 , 0.257 0.191 , 0.254	Depositor DCC
R_{free} test set	7055 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27379	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z98, B12, 5AD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.95	4/5756 (0.1%)	1.01	8/7794 (0.1%)
1	B	1.03	3/5777 (0.1%)	1.04	8/7818 (0.1%)
1	C	0.93	2/5759 (0.0%)	0.99	8/7796 (0.1%)
1	D	1.04	5/5769 (0.1%)	1.02	4/7808 (0.1%)
2	E	0.89	0/867	0.95	1/1163 (0.1%)
2	F	1.08	0/870	1.08	0/1167
2	G	0.81	0/867	1.02	0/1163
2	H	0.97	0/867	0.97	1/1163 (0.1%)
All	All	0.98	14/26532 (0.1%)	1.02	30/35872 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	GLY	C-O	-8.06	1.18	1.24
1	A	326	THR	CA-C	7.54	1.56	1.52
1	D	194	ILE	CA-CB	-7.37	1.46	1.54
1	B	223	GLY	C-O	-7.24	1.19	1.24
1	D	326	THR	CA-C	6.23	1.55	1.52
1	D	218	ILE	C-O	-6.17	1.16	1.24
1	B	218	ILE	C-O	-5.96	1.17	1.24
1	A	218	ILE	C-O	-5.89	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	284	ALA	CA-CB	-5.79	1.44	1.53
1	A	219	ASP	C-O	-5.74	1.16	1.24
1	D	219	ASP	C-O	-5.62	1.17	1.23
1	A	362	MET	N-CA	-5.55	1.39	1.46
1	B	219	ASP	C-O	-5.33	1.18	1.23
1	C	218	ILE	C-O	-5.01	1.18	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	647	VAL	CA-C-N	-8.31	111.46	119.85
1	C	647	VAL	C-N-CA	-8.31	111.46	119.85
1	C	683	ILE	CB-CA-C	-7.66	101.98	112.24
1	B	629	LYS	N-CA-C	7.01	119.52	111.11
1	B	342	VAL	N-CA-C	-6.96	102.54	109.02
1	A	620	VAL	N-CA-C	6.89	117.01	110.53
1	D	7	LEU	N-CA-C	6.38	119.88	110.30
1	D	69	ASP	N-CA-C	6.22	120.00	111.54
1	C	626	ILE	CB-CA-C	-6.08	105.63	111.05
1	B	626	ILE	N-CA-C	5.88	116.62	111.56
1	B	374	GLU	N-CA-C	-5.84	99.76	109.46
1	D	657	ILE	CB-CA-C	-5.81	104.43	112.04
1	A	197	ILE	N-CA-C	-5.72	104.77	111.00
1	C	626	ILE	N-CA-C	5.62	116.06	111.62
1	B	626	ILE	CB-CA-C	-5.47	106.24	111.44
1	A	560	MET	N-CA-C	-5.45	104.22	111.24
2	H	26	PHE	N-CA-C	-5.43	105.44	111.36
1	A	163	GLY	N-CA-C	5.36	119.43	111.76
1	B	619	SER	CA-C-N	5.34	127.29	120.56
1	B	619	SER	C-N-CA	5.34	127.29	120.56
1	D	219	ASP	N-CA-C	5.33	118.11	109.79
1	A	693	ARG	N-CA-C	5.28	117.72	111.33
2	E	6	ASP	N-CA-C	5.21	125.59	111.00
1	C	188	ASN	N-CA-C	5.20	117.35	111.11
1	A	268	PRO	CA-C-N	5.16	124.95	119.28
1	A	268	PRO	C-N-CA	5.16	124.95	119.28
1	A	197	ILE	CB-CA-C	-5.10	105.41	112.24
1	C	187	TYR	N-CA-C	-5.10	105.62	111.07
1	C	267	VAL	CB-CA-C	-5.05	105.18	110.53
1	B	31	GLY	N-CA-C	5.03	116.73	111.95

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	GLN	Peptide
1	D	6	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5651	0	5584	164	0
1	B	5672	0	5644	185	0
1	C	5654	0	5621	182	0
1	D	5664	0	5636	161	0
2	E	855	0	863	17	0
2	F	858	0	865	24	0
2	G	855	0	863	23	0
2	H	855	0	863	16	0
3	A	91	0	87	17	0
3	B	91	0	87	20	0
3	C	91	0	87	16	0
3	D	91	0	87	14	0
4	A	18	0	11	2	0
4	B	18	0	12	2	0
4	C	18	0	12	3	0
4	D	18	0	12	4	0
5	A	23	0	14	11	0
5	B	23	0	14	8	0
5	C	23	0	14	8	0
5	D	23	0	14	8	0
6	A	144	0	0	8	0
6	B	199	0	0	14	0
6	C	145	0	0	14	0
6	D	217	0	0	20	0
6	E	15	0	0	1	0
6	F	33	0	0	2	0
6	G	17	0	0	2	0
6	H	17	0	0	1	0
All	All	27379	0	26390	782	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (782) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:767:Z98:H4A	1:D:629:LYS:NZ	1.46	1.28
1:B:649:VAL:HG22	1:B:683:ILE:HD11	1.20	1.17
1:A:629:LYS:NZ	5:C:767:Z98:H4A	1.64	1.12
1:B:396:ILE:HD12	2:F:29:MET:HE3	1.26	1.12
2:F:54:LEU:HD23	2:F:57:MET:CE	1.78	1.12
3:C:1801:B12:H362	3:C:1801:B12:H351	1.30	1.11
3:B:1801:B12:H362	3:B:1801:B12:H351	1.29	1.11
1:D:445:MET:HE1	1:D:447:PRO:HB3	1.30	1.11
1:B:649:VAL:CG2	1:B:683:ILE:HD11	1.79	1.10
1:B:629:LYS:NZ	5:D:767:Z98:C4A	2.14	1.10
1:D:41:LEU:HD23	1:D:43:MET:HE2	1.19	1.10
1:A:41:LEU:HD21	1:A:43:MET:HE2	1.29	1.09
1:C:41:LEU:HD23	1:C:43:MET:HE2	1.23	1.09
3:D:1801:B12:H362	3:D:1801:B12:H351	1.27	1.09
1:C:41:LEU:CD2	1:C:43:MET:HE2	1.83	1.09
1:B:649:VAL:HG13	1:B:683:ILE:CD1	1.82	1.09
5:A:767:Z98:H4A	1:C:629:LYS:CE	1.83	1.06
3:A:1801:B12:H362	3:A:1801:B12:H351	1.31	1.06
1:B:649:VAL:CG1	1:B:683:ILE:CD1	2.34	1.05
1:A:41:LEU:CD2	1:A:43:MET:HE2	1.86	1.05
1:C:41:LEU:HD23	1:C:43:MET:CE	1.87	1.04
1:B:445:MET:HE1	1:B:447:PRO:HB3	1.38	1.04
5:B:767:Z98:H4A	1:D:629:LYS:CE	1.86	1.04
1:B:649:VAL:CG1	1:B:683:ILE:HD12	1.88	1.00
5:B:767:Z98:C4A	1:D:629:LYS:NZ	2.26	0.99
1:B:649:VAL:HG22	1:B:683:ILE:CD1	1.93	0.98
1:B:649:VAL:CG2	1:B:683:ILE:CD1	2.42	0.97
2:H:54:LEU:HD23	2:H:57:MET:HE2	1.46	0.97
1:B:153:ARG:HD2	6:B:783:HOH:O	1.63	0.97
3:B:1801:B12:H531	3:B:1801:B12:H552	1.45	0.97
1:A:629:LYS:NZ	5:C:767:Z98:C4A	2.28	0.97
1:B:629:LYS:CE	5:D:767:Z98:H4A	1.95	0.97
1:B:172:MET:C	1:B:172:MET:CE	2.38	0.96
5:A:767:Z98:C4A	1:C:629:LYS:NZ	2.29	0.96
2:F:54:LEU:HD23	2:F:57:MET:HE2	1.44	0.95
5:A:767:Z98:H4A	1:C:629:LYS:NZ	1.83	0.94
1:C:406:GLU:OE2	1:C:428:ILE:HG22	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:VAL:HG12	1:A:686:LEU:HD12	1.48	0.93
1:B:649:VAL:HG11	1:B:683:ILE:HD12	1.50	0.93
1:D:41:LEU:CD2	1:D:43:MET:HE2	1.99	0.93
5:B:767:Z98:H4A	1:D:629:LYS:HZ3	1.33	0.92
1:A:172:MET:HE3	1:A:176:GLU:HG3	1.51	0.92
1:B:445:MET:HE1	1:B:447:PRO:CB	2.00	0.91
1:B:629:LYS:HZ3	5:D:767:Z98:C4A	1.83	0.91
1:B:396:ILE:HD12	2:F:29:MET:CE	2.01	0.91
1:B:172:MET:HE2	1:B:173:PHE:N	1.85	0.90
1:C:445:MET:HE1	1:C:447:PRO:CA	2.00	0.90
1:A:445:MET:HE1	1:A:447:PRO:HB3	1.51	0.90
2:F:54:LEU:HD23	2:F:57:MET:HE1	1.54	0.90
1:C:445:MET:HE1	1:C:447:PRO:HB3	1.54	0.89
1:A:668:THR:HG21	1:A:676:HIS:HA	1.53	0.88
1:B:172:MET:C	1:B:172:MET:HE3	1.98	0.88
1:B:629:LYS:NZ	5:D:767:Z98:H4A	1.88	0.88
1:C:445:MET:HE1	1:C:447:PRO:CB	2.04	0.88
1:B:172:MET:C	1:B:172:MET:HE2	1.98	0.87
5:A:767:Z98:C4A	1:C:629:LYS:HZ1	1.84	0.87
1:C:15:VAL:CG2	1:C:499:MET:HE1	2.05	0.87
1:C:15:VAL:HG23	1:C:499:MET:HE1	1.55	0.87
1:C:240:GLU:OE2	1:C:244:GLN:NE2	2.07	0.87
1:D:445:MET:HE3	1:D:471:LEU:HD23	1.56	0.86
1:D:172:MET:C	1:D:172:MET:CE	2.48	0.86
1:A:15:VAL:HG13	1:A:499:MET:HE1	1.56	0.86
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.57	0.85
5:B:767:Z98:C4A	1:D:629:LYS:HZ3	1.89	0.85
1:B:15:VAL:HG23	1:B:499:MET:HE1	1.57	0.85
2:H:54:LEU:HD23	2:H:57:MET:CE	2.06	0.85
1:A:606:LEU:HD21	1:A:732:LEU:HD13	1.57	0.85
3:D:1801:B12:H351	3:D:1801:B12:C36	2.07	0.83
1:D:301:ASN:O	1:D:305:MET:CE	2.27	0.83
1:B:629:LYS:HZ1	5:D:767:Z98:C4A	1.88	0.83
5:B:767:Z98:H4A	1:D:629:LYS:HZ1	1.39	0.83
3:B:1801:B12:H362	3:B:1801:B12:C35	2.06	0.82
1:C:406:GLU:CD	1:C:428:ILE:HG22	2.04	0.82
1:D:172:MET:C	1:D:172:MET:HE3	2.04	0.82
1:A:629:LYS:HZ3	5:C:767:Z98:C4A	1.90	0.82
1:B:541:ILE:HD11	1:B:554:VAL:HG23	1.61	0.82
2:G:54:LEU:HD23	2:G:57:MET:CE	2.10	0.82
1:D:668:THR:HG23	1:D:676:HIS:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:ASN:O	1:C:683:ILE:HG13	1.80	0.80
1:B:123:THR:O	1:B:498:ARG:NH2	2.12	0.80
3:D:1801:B12:H362	3:D:1801:B12:C35	2.11	0.80
1:D:445:MET:HE1	1:D:447:PRO:CB	2.10	0.80
1:B:668:THR:O	1:B:668:THR:CG2	2.29	0.79
3:B:1801:B12:H351	3:B:1801:B12:C36	2.11	0.79
1:B:86:ARG:NE	1:B:125:GLN:HE22	1.80	0.79
1:D:607:LYS:O	1:D:608:ILE:HD12	1.81	0.79
3:D:1801:B12:H552	3:D:1801:B12:H531	1.65	0.79
1:B:396:ILE:CD1	2:F:29:MET:HE3	2.11	0.79
1:B:649:VAL:CG1	1:B:683:ILE:HD11	2.12	0.79
3:A:1801:B12:H351	3:A:1801:B12:C36	2.10	0.79
1:A:629:LYS:HZ1	5:C:767:Z98:H4A	1.43	0.78
5:A:767:Z98:H4A	1:C:629:LYS:HE2	1.65	0.78
1:D:233:GLU:OE1	1:D:236:LYS:NZ	2.16	0.78
1:B:649:VAL:HG13	1:B:683:ILE:HD11	1.65	0.78
1:B:19:LEU:HD12	1:B:499:MET:HE2	1.66	0.77
1:B:608:ILE:HG13	1:B:663:ALA:HB3	1.66	0.77
1:A:445:MET:HE1	1:A:447:PRO:CB	2.14	0.77
1:C:301:ASN:HD21	1:C:304:TYR:H	1.31	0.77
1:B:172:MET:HE3	1:B:172:MET:O	1.84	0.77
1:B:445:MET:HE1	1:B:447:PRO:CA	2.14	0.76
1:B:668:THR:CG2	1:B:676:HIS:HB2	2.15	0.76
1:A:629:LYS:HZ1	5:C:767:Z98:C4A	1.97	0.75
1:D:41:LEU:HD23	1:D:43:MET:CE	2.10	0.75
3:A:1801:B12:H362	3:A:1801:B12:C35	2.16	0.75
2:F:54:LEU:HA	2:F:57:MET:HE2	1.68	0.75
1:A:629:LYS:CE	5:C:767:Z98:H4A	2.15	0.75
1:D:172:MET:C	1:D:172:MET:HE2	2.12	0.75
2:F:68:VAL:HG12	2:F:72:MET:HE2	1.69	0.74
1:C:537:GLU:HG3	1:C:554:VAL:HG21	1.69	0.74
1:B:649:VAL:HG13	1:B:683:ILE:CG1	2.17	0.74
1:A:403:ASN:O	1:A:407:GLN:HG3	1.87	0.74
1:A:461:ASP:CG	1:A:464:LEU:HD13	2.11	0.74
1:B:649:VAL:CB	1:B:683:ILE:HD11	2.18	0.74
1:D:238:MET:SD	6:D:831:HOH:O	2.46	0.73
1:D:172:MET:HE3	1:D:172:MET:O	1.88	0.73
1:D:668:THR:CG2	1:D:676:HIS:HB2	2.18	0.73
2:G:54:LEU:HA	2:G:57:MET:HE2	1.70	0.73
1:A:302:THR:CG2	1:A:334:ILE:HD12	2.19	0.73
1:A:43:MET:HE1	6:A:803:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:767:Z98:H5A	6:A:919:HOH:O	1.89	0.72
1:D:592:LEU:HD22	6:D:960:HOH:O	1.89	0.72
1:D:158:HIS:CE1	1:D:218:ILE:HD12	2.25	0.72
2:F:54:LEU:CD2	2:F:57:MET:CE	2.64	0.71
1:D:235:TRP:C	6:D:831:HOH:O	2.33	0.71
1:C:47:ILE:HG21	6:C:900:HOH:O	1.89	0.71
1:C:525:LEU:HD21	1:C:547:MET:HE1	1.72	0.71
1:B:738:GLU:O	1:B:738:GLU:HG3	1.91	0.71
1:D:740:ARG:C	6:D:845:HOH:O	2.33	0.71
2:F:57:MET:HE1	2:F:82:GLY:HA2	1.72	0.70
1:C:26:THR:HG22	1:C:27:PRO:HD2	1.74	0.70
1:A:464:LEU:HD22	1:A:471:LEU:CD1	2.21	0.70
1:C:445:MET:CE	1:C:447:PRO:CA	2.70	0.70
1:C:96:MET:HE1	1:C:345:HIS:HB3	1.73	0.70
1:C:445:MET:HE2	1:C:446:ALA:C	2.16	0.70
1:C:649:VAL:HG12	1:C:686:LEU:HD12	1.73	0.70
1:C:479:VAL:HG12	1:C:479:VAL:O	1.92	0.69
1:C:251:PHE:O	1:C:255:VAL:HG23	1.92	0.69
2:G:57:MET:HE1	2:G:82:GLY:HA2	1.74	0.69
1:D:301:ASN:O	1:D:305:MET:HE3	1.91	0.69
3:C:1801:B12:H362	3:C:1801:B12:C35	2.16	0.69
2:F:10:ARG:HD2	6:F:823:HOH:O	1.92	0.68
1:D:711:VAL:HG12	1:D:711:VAL:O	1.93	0.68
3:C:1801:B12:H351	3:C:1801:B12:C36	2.11	0.68
1:B:668:THR:HG21	1:B:676:HIS:HB2	1.75	0.68
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.76	0.68
1:A:5:LEU:O	1:A:6:GLN:HB2	1.93	0.68
1:A:577:SER:O	1:A:578:ILE:HD12	1.94	0.68
1:A:178:VAL:O	1:A:215:MET:HE3	1.94	0.67
1:B:668:THR:HG23	1:B:676:HIS:CB	2.24	0.67
1:C:305:MET:HE2	6:C:829:HOH:O	1.94	0.67
1:B:668:THR:O	1:B:668:THR:HG23	1.94	0.67
1:D:389:VAL:HG13	2:H:29:MET:HE1	1.77	0.67
2:F:62:LEU:HD23	6:F:429:HOH:O	1.94	0.67
1:D:172:MET:HE1	1:D:173:PHE:HD1	1.60	0.67
1:B:649:VAL:HG13	1:B:683:ILE:HG13	1.77	0.67
1:D:302:THR:HA	1:D:305:MET:HE3	1.76	0.67
1:C:389:VAL:HG13	2:G:29:MET:HE1	1.76	0.66
1:A:5:LEU:O	1:A:5:LEU:HD23	1.96	0.66
1:C:406:GLU:OE2	1:C:428:ILE:CG2	2.43	0.66
1:B:233:GLU:HG2	1:B:235:TRP:CH2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:CB	6:A:911:HOH:O	2.44	0.66
1:A:234:ALA:O	1:A:237:VAL:HG12	1.96	0.66
1:B:629:LYS:HZ3	5:D:767:Z98:C4	2.09	0.66
5:B:767:Z98:H4A	1:D:629:LYS:HE2	1.75	0.66
1:A:703:THR:HG22	1:A:704:GLN:HE21	1.59	0.66
1:C:41:LEU:HD21	1:C:43:MET:HE2	1.76	0.66
1:C:305:MET:CE	6:C:829:HOH:O	2.43	0.66
1:C:608:ILE:HD11	1:C:663:ALA:HB3	1.78	0.66
1:C:597:ILE:CD1	1:C:726:ILE:CD1	2.74	0.65
3:A:1801:B12:N29	3:A:1801:B12:H251	2.09	0.65
1:D:172:MET:CE	1:D:173:PHE:HD1	2.08	0.65
1:B:73:GLN:NE2	1:B:153:ARG:HH22	1.94	0.65
1:A:41:LEU:HD23	1:A:43:MET:HE2	1.76	0.65
1:A:172:MET:HE3	1:A:176:GLU:CG	2.24	0.65
2:F:54:LEU:CD2	2:F:57:MET:HE1	2.26	0.65
1:C:207:LYS:NZ	1:C:217:GLN:HE22	1.95	0.65
1:D:172:MET:HE2	1:D:173:PHE:N	2.11	0.65
1:B:92:ARG:HD2	6:D:841:HOH:O	1.97	0.64
1:B:86:ARG:HE	1:B:125:GLN:NE2	1.95	0.64
1:C:723:SER:O	3:C:1801:B12:O8R	2.16	0.64
1:D:120:ILE:HG13	1:D:133:THR:HG22	1.77	0.64
1:A:445:MET:HE1	1:A:447:PRO:CA	2.27	0.64
1:B:149:GLU:HG2	6:B:795:HOH:O	1.98	0.64
1:D:464:LEU:HD23	1:D:471:LEU:HD13	1.78	0.64
1:B:86:ARG:HE	1:B:125:GLN:HE22	1.46	0.64
1:D:429:ASN:HB3	6:D:873:HOH:O	1.98	0.64
1:C:475:CYS:HB2	2:G:56:ARG:O	1.98	0.64
1:A:568:ILE:HG22	1:A:570:LEU:CD1	2.28	0.64
3:B:1801:B12:N23	4:D:1500:5AD:H4'	2.13	0.64
1:B:171:VAL:HG23	1:B:209:ILE:HD13	1.80	0.63
1:A:153:ARG:HD2	6:A:783:HOH:O	1.97	0.63
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.80	0.63
1:D:649:VAL:HG23	6:D:943:HOH:O	1.96	0.63
1:B:301:ASN:O	1:B:305:MET:CE	2.46	0.63
1:B:541:ILE:CD1	1:B:554:VAL:HG23	2.27	0.63
2:H:25:ARG:HA	2:H:28:GLU:HG2	1.80	0.63
1:A:697:MET:HE1	1:A:736:ARG:HB2	1.79	0.63
1:B:43:MET:CE	1:B:72:PRO:HB3	2.28	0.63
1:B:88:GLU:OE2	1:B:498:ARG:HD2	1.99	0.63
1:B:172:MET:CE	1:B:173:PHE:N	2.54	0.63
1:B:246:ALA:O	1:B:250:ILE:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:ARG:HD3	6:D:849:HOH:O	1.99	0.63
1:C:335:THR:HG22	1:C:348:ASN:HA	1.81	0.63
1:B:7:LEU:HB2	6:B:940:HOH:O	1.98	0.63
1:C:660:LYS:O	1:C:660:LYS:HG3	1.98	0.62
1:C:238:MET:HE3	1:C:283:TYR:HB2	1.82	0.62
1:C:445:MET:HE1	1:C:447:PRO:HA	1.81	0.62
1:D:668:THR:CG2	1:D:668:THR:O	2.47	0.62
1:B:7:LEU:CD2	1:B:146:LEU:HB3	2.29	0.62
1:B:73:GLN:HE21	1:B:153:ARG:HH22	1.46	0.61
3:A:1801:B12:N22	4:C:1500:5AD:H5'1	2.13	0.61
2:H:54:LEU:HA	2:H:57:MET:HE2	1.81	0.61
1:A:629:LYS:HZ3	5:C:767:Z98:H4A	1.51	0.61
1:A:43:MET:HE1	1:A:72:PRO:HA	1.82	0.61
1:B:86:ARG:NE	1:B:125:GLN:NE2	2.48	0.61
3:B:1801:B12:H492	3:B:1801:B12:C47	2.30	0.61
1:C:13:LEU:HD22	1:C:18:ILE:HD11	1.81	0.61
1:C:597:ILE:CD1	1:C:726:ILE:HD11	2.31	0.61
1:A:464:LEU:CD2	1:A:471:LEU:HD13	2.31	0.61
1:C:79:THR:HG21	1:C:106:MET:HE3	1.82	0.61
1:C:123:THR:O	1:C:498:ARG:NH2	2.32	0.61
1:C:153:ARG:HD2	6:C:791:HOH:O	1.99	0.61
1:C:615:GLU:C	6:C:806:HOH:O	2.43	0.61
2:G:54:LEU:HD23	2:G:57:MET:HE2	1.81	0.61
1:A:568:ILE:HG22	1:A:570:LEU:HD12	1.83	0.61
1:B:19:LEU:CD1	1:B:499:MET:HE2	2.31	0.61
1:C:207:LYS:HZ2	1:C:217:GLN:HE22	1.47	0.61
2:G:94:ILE:HD12	2:G:98:GLU:HB3	1.83	0.61
1:B:511:ILE:CG2	1:B:580:ILE:HD11	2.30	0.60
1:B:511:ILE:HG21	1:B:580:ILE:HD11	1.83	0.60
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.37	0.60
1:D:574:VAL:HG13	1:D:576:PHE:CE1	2.36	0.60
3:B:1801:B12:H492	3:B:1801:B12:H473	1.83	0.60
1:C:626:ILE:O	1:C:634:GLU:HB2	2.01	0.60
1:D:344:TRP:O	1:D:345:HIS:C	2.41	0.60
1:C:445:MET:HE3	1:C:471:LEU:HD23	1.83	0.60
1:C:616:ASP:N	6:C:806:HOH:O	2.33	0.60
5:B:767:Z98:C4A	1:D:629:LYS:HZ1	2.05	0.60
1:B:80:THR:OG1	1:B:348:ASN:ND2	2.30	0.60
1:C:7:LEU:HD21	1:C:95:ARG:NH2	2.16	0.60
1:A:606:LEU:HD12	1:A:662:ASP:OD2	2.01	0.60
1:B:39:GLU:OE1	1:B:39:GLU:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:MET:HE1	1:B:72:PRO:HA	1.84	0.60
2:H:98:GLU:HG3	6:H:490:HOH:O	2.02	0.60
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.32	0.59
1:B:41:LEU:HD23	1:B:43:MET:HE2	1.85	0.59
1:D:210:MET:HE3	1:D:215:MET:HE2	1.84	0.59
1:A:703:THR:O	1:A:721:ARG:NH1	2.35	0.59
1:B:509:SER:N	6:B:925:HOH:O	2.35	0.59
3:B:1801:B12:H203	3:B:1801:B12:H301	1.84	0.59
1:A:664:ILE:O	1:A:665:LEU:HD23	2.03	0.59
1:B:43:MET:HE1	1:B:72:PRO:HB3	1.85	0.59
1:C:445:MET:CE	1:C:447:PRO:HA	2.32	0.59
1:D:736:ARG:CD	6:D:849:HOH:O	2.50	0.59
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.37	0.59
1:B:15:VAL:HG22	6:B:913:HOH:O	2.01	0.59
1:C:525:LEU:HB3	1:C:570:LEU:HD12	1.84	0.59
1:A:459:GLN:HG3	1:A:460:TYR:CD2	2.38	0.59
1:D:445:MET:CE	1:D:471:LEU:HD23	2.28	0.59
1:B:513:PRO:O	1:B:521:GLY:HA2	2.03	0.58
3:C:1801:B12:H552	3:C:1801:B12:H531	1.83	0.58
1:D:427:GLN:HG3	6:D:824:HOH:O	2.03	0.58
1:A:79:THR:HB	1:A:332:SER:HA	1.86	0.58
1:B:689:GLU:O	1:B:689:GLU:HG2	2.04	0.58
1:B:738:GLU:O	1:B:738:GLU:CG	2.51	0.58
1:C:202:ASP:OD2	2:G:48:SER:OG	2.16	0.58
1:D:160:TYR:OH	5:D:767:Z98:HB	2.04	0.58
1:A:726:ILE:HG23	1:A:727:HIS:CD2	2.38	0.58
1:C:668:THR:HG23	1:C:676:HIS:CB	2.32	0.58
1:D:607:LYS:C	1:D:608:ILE:HD12	2.28	0.58
1:D:680:MET:HE1	1:D:705:VAL:HG13	1.86	0.58
1:B:18:ILE:O	1:B:142:LYS:NZ	2.33	0.58
1:A:608:ILE:HD13	1:A:638:VAL:CG1	2.34	0.58
1:D:389:VAL:HG13	2:H:29:MET:CE	2.33	0.58
1:C:290:MET:HE2	1:C:385:LYS:HG2	1.86	0.58
1:A:302:THR:HG21	1:A:334:ILE:HD12	1.86	0.57
1:A:580:ILE:CD1	1:C:535:VAL:HG11	2.34	0.57
1:A:546:LYS:HZ2	1:C:578:ILE:HD11	1.69	0.57
1:B:540:ALA:HB1	1:B:570:LEU:HD11	1.85	0.57
1:B:82:ILE:HG22	1:B:90:ASP:HB3	1.85	0.57
1:C:687:ALA:HB3	1:C:693:ARG:HD3	1.85	0.57
1:D:668:THR:HG23	1:D:676:HIS:CB	2.30	0.57
1:A:200:PHE:CD2	2:E:37:LEU:HD13	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:O	1:B:494:ASN:HA	2.05	0.57
1:C:596:GLU:CB	6:C:826:HOH:O	2.52	0.57
1:B:415:TYR:O	1:B:416:TYR:C	2.48	0.57
1:C:445:MET:CE	1:C:447:PRO:N	2.67	0.57
1:D:608:ILE:HG13	1:D:663:ALA:HB3	1.86	0.57
1:A:164:VAL:HG13	1:A:194:ILE:HG12	1.87	0.57
1:A:464:LEU:CD2	1:A:471:LEU:CD1	2.83	0.57
1:B:266:THR:O	1:B:266:THR:HG23	2.03	0.57
1:B:668:THR:O	1:B:668:THR:HG22	2.04	0.57
1:A:41:LEU:CD2	1:A:43:MET:CE	2.74	0.57
4:B:1500:5AD:C4'	3:D:1801:B12:N23	2.67	0.57
1:B:629:LYS:HE2	5:D:767:Z98:H4A	1.81	0.57
1:B:416:TYR:CD1	1:B:417:PRO:HA	2.40	0.56
1:B:445:MET:HA	1:B:455:ASN:OD1	2.05	0.56
1:B:668:THR:CG2	1:B:676:HIS:CB	2.80	0.56
1:C:234:ALA:O	1:C:237:VAL:HG12	2.06	0.56
1:C:537:GLU:CG	1:C:554:VAL:HG21	2.35	0.56
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.87	0.56
1:B:393:GLU:OE2	2:F:25:ARG:NH1	2.32	0.56
1:B:504:GLU:CB	6:B:840:HOH:O	2.52	0.56
1:B:445:MET:CE	1:B:471:LEU:HD23	2.35	0.56
1:C:7:LEU:HD22	1:C:150:GLU:OE2	2.05	0.56
1:C:233:GLU:HG2	1:C:235:TRP:CH2	2.41	0.56
1:A:269:PRO:HB2	1:A:270:THR:HG23	1.89	0.56
1:A:613:VAL:HG21	1:A:649:VAL:CG2	2.36	0.56
1:C:428:ILE:HG21	6:C:778:HOH:O	2.06	0.56
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.41	0.55
1:B:120:ILE:HG13	1:B:133:THR:HG22	1.87	0.55
1:C:612:THR:HB	1:C:645:THR:HG22	1.89	0.55
1:D:591:ILE:HG23	1:D:591:ILE:O	2.05	0.55
1:C:13:LEU:CD2	1:C:18:ILE:HD11	2.37	0.55
3:B:1801:B12:C35	3:B:1801:B12:C36	2.79	0.55
1:D:509:SER:N	6:D:988:HOH:O	2.40	0.55
1:D:610:ALA:HA	1:D:665:LEU:O	2.06	0.55
3:B:1801:B12:O28	3:B:1801:B12:H3	2.06	0.55
1:C:181:ALA:HB3	1:C:210:MET:HE3	1.88	0.55
2:G:54:LEU:HD23	2:G:57:MET:HE1	1.88	0.55
1:D:445:MET:HE2	1:D:447:PRO:CA	2.36	0.55
1:D:574:VAL:CG1	1:D:576:PHE:CE1	2.90	0.55
1:B:607:LYS:C	1:B:608:ILE:HD12	2.32	0.55
1:C:15:VAL:HG21	1:C:499:MET:HE1	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:PRO:O	1:D:736:ARG:NH2	2.39	0.55
3:D:1801:B12:H492	3:D:1801:B12:C47	2.36	0.55
1:A:392:MET:HE2	2:E:26:PHE:CE1	2.42	0.55
1:B:207:LYS:NZ	1:B:217:GLN:NE2	2.55	0.55
1:C:594:GLU:CB	6:C:819:HOH:O	2.55	0.55
1:D:305:MET:HE1	1:D:334:ILE:HG21	1.89	0.55
1:D:445:MET:HE2	1:D:447:PRO:N	2.22	0.55
1:C:161:VAL:HG12	1:C:161:VAL:O	2.06	0.55
1:B:301:ASN:O	1:B:305:MET:HE3	2.06	0.54
3:A:1801:B12:H552	3:A:1801:B12:H531	1.89	0.54
1:D:449:THR:OG1	1:D:478:GLU:OE2	2.16	0.54
1:A:613:VAL:HG21	1:A:649:VAL:HG23	1.89	0.54
4:A:1500:5AD:C4'	3:C:1801:B12:N23	2.70	0.54
1:B:580:ILE:HD13	1:B:580:ILE:N	2.22	0.54
1:A:464:LEU:HD23	1:A:471:LEU:HD13	1.89	0.54
2:E:6:ASP:N	6:E:410:HOH:O	2.40	0.54
1:A:543:PHE:CE1	1:C:578:ILE:HD13	2.42	0.54
1:A:392:MET:CE	2:E:30:ALA:HB2	2.38	0.54
1:B:649:VAL:CB	1:B:683:ILE:CD1	2.83	0.54
1:D:26:THR:HG22	1:D:27:PRO:HD2	1.88	0.54
1:D:510:MET:HE3	1:D:577:SER:HB3	1.90	0.54
2:E:74:ARG:HD2	2:E:113:ILE:HD11	1.88	0.54
1:D:269:PRO:HD2	1:D:280:ASP:CG	2.33	0.54
1:B:668:THR:HG23	1:B:676:HIS:HB3	1.87	0.54
3:B:1801:B12:H531	3:B:1801:B12:C55	2.22	0.53
2:E:53:VAL:O	2:E:57:MET:HG3	2.09	0.53
1:C:445:MET:CE	1:C:471:LEU:HD23	2.39	0.53
1:D:210:MET:HG2	1:D:215:MET:HE2	1.90	0.53
1:A:41:LEU:HD23	1:A:43:MET:CE	2.38	0.53
1:B:238:MET:HE2	1:B:269:PRO:HG2	1.91	0.53
1:A:7:LEU:HB2	6:A:834:HOH:O	2.08	0.53
1:A:53:THR:HG23	1:A:54:PRO:HD2	1.90	0.53
1:B:506:ARG:HH11	1:B:518:GLN:HE22	1.56	0.53
1:B:610:ALA:HB1	1:B:622:LEU:HD21	1.91	0.53
1:C:82:ILE:HG22	1:C:90:ASP:HB3	1.90	0.53
2:G:7:PHE:CZ	2:G:11:ARG:HD2	2.43	0.53
1:A:369:VAL:CG1	1:C:369:VAL:CG1	2.87	0.53
1:A:728:VAL:HG21	3:A:1801:B12:HM62	1.91	0.53
1:C:7:LEU:CD2	1:C:95:ARG:NH2	2.72	0.53
1:A:5:LEU:O	1:A:6:GLN:CB	2.56	0.53
1:A:713:GLN:HA	1:A:713:GLN:HE21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:LYS:NZ	6:C:815:HOH:O	2.31	0.53
1:D:606:LEU:HD11	1:D:608:ILE:HD11	1.91	0.53
1:B:364:GLY:O	1:B:365:LEU:C	2.49	0.53
1:B:629:LYS:NZ	1:D:226:ASN:OD1	2.40	0.53
1:D:445:MET:CE	1:D:447:PRO:CA	2.87	0.53
1:C:6:GLN:HG2	1:C:7:LEU:N	2.24	0.53
1:D:399:GLY:HA3	1:D:403:ASN:HD22	1.73	0.53
1:D:669:ILE:N	1:D:669:ILE:HD13	2.24	0.53
1:C:232:ARG:HA	1:C:232:ARG:HH11	1.74	0.52
1:A:126:GLY:O	1:A:127:ILE:HD13	2.10	0.52
2:F:86:TYR:O	2:F:89:ALA:HB3	2.09	0.52
1:A:123:THR:O	1:A:498:ARG:NH2	2.42	0.52
1:C:415:TYR:O	1:C:416:TYR:C	2.53	0.52
1:A:370:GLN:NE2	1:C:370:GLN:OE1	2.40	0.52
1:B:149:GLU:CG	6:B:795:HOH:O	2.56	0.52
1:D:596:GLU:CB	6:D:960:HOH:O	2.56	0.52
1:A:392:MET:HE1	2:E:30:ALA:HB2	1.92	0.52
1:C:392:MET:HE1	2:G:30:ALA:HB2	1.92	0.52
3:A:1801:B12:C6	4:C:1500:5AD:H5'1	2.39	0.52
1:A:134:ARG:NH1	1:A:175:GLU:OE2	2.34	0.52
1:A:623:ARG:HD3	1:C:115:HIS:CE1	2.44	0.52
1:C:7:LEU:HD12	1:C:146:LEU:HB3	1.91	0.52
1:D:123:THR:O	1:D:498:ARG:NH2	2.42	0.52
1:A:162:SER:OG	5:A:767:Z98:N1	2.37	0.52
1:B:267:VAL:HG22	1:B:299:GLN:HB3	1.91	0.52
4:B:1500:5AD:H4'	3:D:1801:B12:N23	2.25	0.52
1:A:709:VAL:O	1:A:712:LYS:HB3	2.09	0.52
1:B:43:MET:HE1	1:B:72:PRO:CA	2.40	0.52
1:A:710:ALA:O	1:A:715:VAL:HG23	2.10	0.51
1:B:234:ALA:O	1:B:237:VAL:HG12	2.10	0.51
1:C:392:MET:CE	2:G:30:ALA:HB2	2.39	0.51
2:G:20:GLU:HB3	6:G:725:HOH:O	2.10	0.51
2:E:92:LYS:HB2	2:E:94:ILE:HG12	1.92	0.51
1:D:172:MET:HE1	1:D:173:PHE:CD1	2.44	0.51
1:A:57:ASN:HB3	1:A:99:TRP:CH2	2.45	0.51
1:B:628:ILE:HD12	1:D:424:ILE:HD11	1.92	0.51
1:C:445:MET:HE3	1:C:471:LEU:CD2	2.39	0.51
1:C:580:ILE:HG22	1:C:580:ILE:O	2.11	0.51
5:A:767:Z98:H4A	1:C:629:LYS:HZ1	1.57	0.51
1:D:340:ARG:HG2	1:D:555:ILE:HD12	1.93	0.51
1:A:201:ILE:HD13	2:E:44:ASN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LYS:NZ	1:B:217:GLN:HE22	2.09	0.51
1:C:608:ILE:CD1	1:C:663:ALA:HB3	2.39	0.51
4:A:1500:5AD:H4'	3:C:1801:B12:N23	2.24	0.51
1:A:200:PHE:CE2	2:E:37:LEU:HD13	2.45	0.51
2:E:85:VAL:HG22	2:E:103:LEU:HD12	1.93	0.51
2:F:55:LEU:HD23	2:F:59:PHE:O	2.11	0.51
1:C:207:LYS:NZ	1:C:217:GLN:NE2	2.59	0.51
1:B:541:ILE:HD12	1:B:552:VAL:HG12	1.93	0.51
2:F:103:LEU:HD23	2:F:107:LYS:O	2.11	0.51
1:C:660:LYS:O	1:C:660:LYS:CG	2.59	0.51
1:A:94:MET:HE2	1:A:105:ILE:HG21	1.93	0.51
1:A:694:ASP:OD1	1:A:694:ASP:C	2.54	0.51
1:D:266:THR:O	1:D:266:THR:HG23	2.10	0.51
3:A:1801:B12:N23	4:C:1500:5AD:H4'	2.26	0.50
2:E:20:GLU:H	2:E:20:GLU:CD	2.18	0.50
2:F:45:THR:OG1	2:F:46:THR:N	2.43	0.50
1:C:506:ARG:HH11	1:C:518:GLN:HE22	1.60	0.50
1:A:87:PHE:HE1	1:A:139:ALA:CB	2.23	0.50
1:A:172:MET:C	1:A:172:MET:HE2	2.36	0.50
2:G:114:GLN:C	6:G:125:HOH:O	2.54	0.50
1:D:541:ILE:CD1	1:D:554:VAL:HG23	2.41	0.50
1:B:43:MET:HE1	1:B:72:PRO:CB	2.41	0.50
1:C:123:THR:HG23	1:C:135:LYS:HD3	1.93	0.50
1:B:445:MET:HE1	1:B:447:PRO:HA	1.93	0.50
1:C:41:LEU:HD23	1:C:43:MET:HE3	1.89	0.50
1:B:668:THR:HG23	1:B:676:HIS:HB2	1.85	0.50
3:D:1801:B12:H252	3:D:1801:B12:H601	1.93	0.50
1:A:289:GLU:CD	1:A:373:ARG:HH21	2.19	0.50
1:A:512:LYS:HB2	1:A:513:PRO:CD	2.42	0.50
1:B:295:ARG:HD3	6:B:898:HOH:O	2.11	0.50
1:D:88:GLU:OE2	1:D:498:ARG:HD2	2.12	0.50
1:A:540:ALA:HB1	1:A:570:LEU:HD11	1.93	0.49
1:B:42:GLN:NE2	1:B:44:GLY:O	2.45	0.49
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.12	0.49
1:D:416:TYR:CG	1:D:417:PRO:HA	2.46	0.49
2:F:95:SER:OG	2:F:98:GLU:HG3	2.12	0.49
1:C:161:VAL:O	1:C:161:VAL:CG1	2.60	0.49
1:C:581:ASN:C	1:C:583:LEU:H	2.20	0.49
1:D:611:ALA:HB1	1:D:647:VAL:HG21	1.94	0.49
1:A:138:ARG:O	1:A:139:ALA:C	2.54	0.49
1:B:233:GLU:HG2	1:B:235:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.94	0.49
1:B:130:VAL:HG13	6:B:774:HOH:O	2.13	0.49
1:D:723:SER:O	3:D:1801:B12:H5R1	2.12	0.49
1:A:710:ALA:O	1:A:715:VAL:CG2	2.61	0.49
1:B:445:MET:CE	1:B:447:PRO:CA	2.90	0.49
1:C:346:ILE:HG23	6:C:891:HOH:O	2.11	0.49
1:D:123:THR:O	1:D:494:ASN:HA	2.12	0.49
3:D:1801:B12:C36	3:D:1801:B12:C35	2.80	0.49
1:A:543:PHE:CZ	1:C:578:ILE:HD13	2.47	0.49
1:B:445:MET:HE2	1:B:446:ALA:C	2.37	0.49
1:D:264:LEU:N	1:D:264:LEU:HD12	2.28	0.49
1:C:213:ALA:HB3	1:C:215:MET:HG3	1.94	0.49
1:D:729:ALA:O	1:D:733:VAL:HG22	2.12	0.49
3:D:1801:B12:C47	3:D:1801:B12:C49	2.91	0.49
1:A:629:LYS:HE2	5:C:767:Z98:H4A	1.94	0.49
1:A:546:LYS:NZ	1:C:578:ILE:HD11	2.28	0.48
1:C:207:LYS:HZ2	1:C:217:GLN:NE2	2.10	0.48
1:B:161:VAL:HG12	1:B:161:VAL:O	2.12	0.48
2:F:110:ASP:O	2:F:114:GLN:HB2	2.13	0.48
1:D:654:ASP:HA	1:D:657:ILE:HD12	1.94	0.48
1:B:250:ILE:O	1:B:251:PHE:C	2.54	0.48
1:B:445:MET:HE3	1:B:471:LEU:CD2	2.44	0.48
1:C:224:ALA:HB3	1:C:245:HIS:CE1	2.48	0.48
1:D:631:GLY:O	1:D:725:GLY:HA3	2.13	0.48
1:A:389:VAL:HG21	2:E:22:LEU:HD11	1.95	0.48
1:D:592:LEU:CD2	6:D:960:HOH:O	2.56	0.48
1:D:654:ASP:OD1	1:D:690:LYS:NZ	2.47	0.48
3:D:1801:B12:H492	3:D:1801:B12:H473	1.95	0.48
1:A:19:LEU:CD1	1:A:499:MET:HE2	2.44	0.48
1:B:204:CYS:HB3	1:B:452:PHE:CD2	2.49	0.48
1:B:506:ARG:HH11	1:B:518:GLN:NE2	2.12	0.48
3:C:1801:B12:O7R	3:C:1801:B12:H2B	2.14	0.48
1:B:224:ALA:HB3	1:B:245:HIS:CE1	2.49	0.48
1:C:616:ASP:HA	6:C:806:HOH:O	2.13	0.48
1:C:649:VAL:CG1	1:C:686:LEU:HD12	2.43	0.48
1:D:13:LEU:HD13	1:D:91:ILE:HG22	1.95	0.48
1:A:238:MET:HA	1:A:241:LEU:HD12	1.95	0.48
1:A:369:VAL:HG13	1:C:369:VAL:CG1	2.44	0.48
1:A:513:PRO:HA	1:C:529:LEU:HD23	1.95	0.48
1:A:608:ILE:HD13	1:A:638:VAL:HG11	1.96	0.48
1:B:526:THR:HG23	1:B:569:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ILE:HD12	1:B:638:VAL:HG11	1.96	0.48
1:D:445:MET:HE2	1:D:446:ALA:C	2.38	0.48
1:D:668:THR:C	1:D:669:ILE:HD13	2.38	0.48
1:A:79:THR:HG21	1:A:106:MET:HE3	1.95	0.48
1:C:132:ILE:HA	1:C:136:GLN:OE1	2.14	0.48
1:A:461:ASP:O	1:A:462:GLU:C	2.56	0.47
1:A:161:VAL:O	1:A:161:VAL:HG12	2.15	0.47
2:F:50:GLU:HG3	2:F:77:MET:HE1	1.96	0.47
1:D:117:ASP:HA	1:D:164:VAL:HG23	1.95	0.47
1:D:711:VAL:O	1:D:711:VAL:CG1	2.59	0.47
1:A:426:ARG:HA	6:A:871:HOH:O	2.13	0.47
1:C:522:THR:HA	1:C:572:GLY:O	2.15	0.47
1:C:616:ASP:CA	6:C:806:HOH:O	2.62	0.47
1:B:377:LEU:O	1:B:381:VAL:HG23	2.15	0.47
1:B:670:ILE:HG23	3:B:1801:B12:O34	2.14	0.47
1:D:79:THR:HA	1:D:104:HIS:HB3	1.97	0.47
1:A:82:ILE:HG22	1:A:90:ASP:HB3	1.96	0.47
1:B:201:ILE:HD13	1:B:437:VAL:HG13	1.97	0.47
2:F:23:GLN:O	2:F:26:PHE:HB3	2.15	0.47
1:C:93:ARG:HA	1:C:96:MET:HE2	1.95	0.47
1:C:94:MET:HE2	1:C:105:ILE:CG2	2.45	0.47
1:C:612:THR:HG22	1:C:616:ASP:HB3	1.96	0.47
1:C:684:HIS:O	1:C:688:VAL:HG23	2.14	0.47
1:D:224:ALA:CB	1:D:245:HIS:CE1	2.98	0.47
2:H:54:LEU:CD2	2:H:57:MET:CE	2.87	0.47
1:A:475:CYS:HB2	2:E:56:ARG:O	2.15	0.47
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.50	0.47
1:B:649:VAL:HG12	1:B:686:LEU:CD1	2.45	0.47
1:C:373:ARG:HA	1:C:377:LEU:HD23	1.97	0.47
1:D:172:MET:CE	1:D:173:PHE:N	2.74	0.47
1:D:269:PRO:HD2	1:D:280:ASP:OD1	2.15	0.47
1:D:290:MET:HE3	2:H:26:PHE:CG	2.49	0.47
1:B:80:THR:HG1	1:B:348:ASN:HD22	1.57	0.47
1:C:26:THR:HG22	1:C:27:PRO:CD	2.43	0.47
1:C:200:PHE:CE2	2:G:37:LEU:HD13	2.50	0.47
1:A:668:THR:HG21	1:A:676:HIS:CA	2.36	0.47
1:C:479:VAL:O	1:C:481:GLU:N	2.48	0.47
1:A:415:TYR:O	1:A:416:TYR:C	2.58	0.46
1:A:485:TYR:C	1:A:486:ILE:HD12	2.40	0.46
1:C:445:MET:HE1	1:C:447:PRO:N	2.29	0.46
1:C:525:LEU:HD21	1:C:547:MET:CE	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:THR:HG22	1:A:348:ASN:HA	1.97	0.46
1:B:233:GLU:CG	1:B:235:TRP:CH2	2.98	0.46
1:B:416:TYR:CG	1:B:417:PRO:HA	2.50	0.46
1:A:459:GLN:HG3	1:A:460:TYR:CE2	2.51	0.46
1:B:428:ILE:CG2	1:B:429:ASN:N	2.78	0.46
1:D:15:VAL:CG2	1:D:499:MET:HE1	2.45	0.46
6:A:768:HOH:O	2:E:87:LYS:CB	2.64	0.46
3:B:1801:B12:C47	3:B:1801:B12:C49	2.90	0.46
1:B:43:MET:HE3	1:B:72:PRO:HB3	1.97	0.46
1:B:528:PHE:C	1:B:528:PHE:CD2	2.93	0.46
1:C:7:LEU:HD21	1:C:95:ARG:CZ	2.45	0.46
1:C:387:ARG:NH1	1:C:416:TYR:O	2.43	0.46
1:D:123:THR:OG1	1:D:495:VAL:HG12	2.16	0.46
1:B:410:PHE:C	1:B:411:VAL:HG23	2.40	0.46
1:B:672:HIS:O	1:B:675:ILE:HG22	2.15	0.46
1:C:189:VAL:HG12	1:C:426:ARG:HG3	1.98	0.46
1:C:416:TYR:CG	1:C:417:PRO:HA	2.51	0.46
1:D:600:ASP:OD2	1:D:736:ARG:NH1	2.49	0.46
2:H:59:PHE:CE1	2:H:100:GLY:HA3	2.51	0.46
1:A:341:ASN:ND2	1:A:342:VAL:O	2.43	0.46
1:B:57:ASN:HB3	1:B:99:TRP:CH2	2.51	0.46
1:C:282:PRO:HG3	1:C:377:LEU:HD12	1.97	0.46
1:C:410:PHE:C	1:C:411:VAL:HG23	2.39	0.46
1:B:158:HIS:HA	1:B:180:GLY:O	2.16	0.46
1:C:444:TYR:CD2	1:C:444:TYR:C	2.93	0.46
1:A:236:LYS:HG2	1:A:415:TYR:HB2	1.98	0.46
1:A:426:ARG:NH1	1:C:634:GLU:OE2	2.31	0.46
1:B:7:LEU:HD23	1:B:146:LEU:HB3	1.96	0.46
1:C:77:VAL:CG1	1:C:104:HIS:HB2	2.46	0.46
3:A:1801:B12:N29	3:A:1801:B12:C25	2.76	0.46
1:B:445:MET:HE3	1:B:471:LEU:HD23	1.97	0.46
1:B:649:VAL:HG21	1:B:683:ILE:CD1	2.39	0.46
1:C:728:VAL:HG21	3:C:1801:B12:HM62	1.98	0.46
3:C:1801:B12:H251	3:C:1801:B12:N29	2.31	0.46
1:D:85:GLY:HA2	1:D:129:GLY:O	2.16	0.45
1:D:649:VAL:HG13	1:D:683:ILE:HG13	1.97	0.45
1:D:606:LEU:CD1	1:D:608:ILE:CD1	2.94	0.45
1:B:607:LYS:O	1:B:608:ILE:HD12	2.17	0.45
1:C:15:VAL:HG23	1:C:16:GLU:N	2.30	0.45
1:D:5:LEU:HD23	1:D:5:LEU:C	2.42	0.45
1:A:344:TRP:CD1	1:A:515:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LYS:NZ	1:C:226:ASN:OD1	2.49	0.45
1:B:268:PRO:HA	1:B:269:PRO:HD3	1.81	0.45
1:C:468:PRO:O	1:C:471:LEU:HB2	2.15	0.45
1:D:267:VAL:HG22	1:D:299:GLN:HB3	1.98	0.45
1:A:75:LEU:N	1:A:76:PRO:CD	2.80	0.45
1:A:649:VAL:O	1:A:653:VAL:HG23	2.16	0.45
1:B:315:THR:HB	6:B:852:HOH:O	2.15	0.45
1:C:305:MET:HE1	1:C:316:HIS:NE2	2.32	0.45
1:D:302:THR:HG23	6:D:973:HOH:O	2.17	0.45
1:A:271:ALA:O	1:A:274:ALA:HB3	2.17	0.45
1:A:504:GLU:HA	6:A:868:HOH:O	2.17	0.45
1:A:723:SER:O	3:A:1801:B12:O8R	2.29	0.45
1:B:90:ASP:O	1:B:94:MET:HG3	2.17	0.45
2:G:53:VAL:O	2:G:57:MET:HG3	2.17	0.45
1:D:82:ILE:HG22	1:D:90:ASP:HB3	1.98	0.45
1:D:593:SER:O	1:D:597:ILE:HG13	2.17	0.45
1:A:138:ARG:HE	1:A:176:GLU:CD	2.25	0.45
1:A:671:SER:HB2	1:A:676:HIS:ND1	2.32	0.45
2:E:54:LEU:HD12	2:E:68:VAL:HG23	1.99	0.45
1:C:8:ARG:HD3	1:C:11:GLU:CD	2.42	0.45
3:C:1801:B12:H252	3:C:1801:B12:H601	1.98	0.45
2:G:50:GLU:HG3	2:G:77:MET:HE1	1.99	0.45
1:D:210:MET:HG2	1:D:215:MET:CE	2.46	0.45
1:D:416:TYR:CD1	1:D:417:PRO:HA	2.52	0.45
2:H:54:LEU:HD23	2:H:57:MET:HE1	1.95	0.45
3:C:1801:B12:C35	3:C:1801:B12:C36	2.84	0.45
2:G:25:ARG:HG2	2:G:29:MET:HE2	1.98	0.45
1:B:729:ALA:O	1:B:733:VAL:HG13	2.17	0.45
1:C:679:ASN:O	1:C:683:ILE:CG1	2.58	0.45
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.52	0.45
1:D:445:MET:CE	1:D:447:PRO:CB	2.88	0.45
3:A:1801:B12:H2B	3:A:1801:B12:O7R	2.17	0.44
1:B:207:LYS:HZ3	1:B:217:GLN:NE2	2.13	0.44
1:B:224:ALA:CB	1:B:245:HIS:CE1	3.00	0.44
2:F:50:GLU:CG	2:F:77:MET:HE1	2.47	0.44
1:C:615:GLU:O	1:C:646:SER:OG	2.34	0.44
1:A:609:VAL:HG21	1:A:656:ALA:HB2	1.99	0.44
1:D:459:GLN:HE22	2:H:83:HIS:CE1	2.35	0.44
1:A:542:GLU:HG3	1:C:583:LEU:CD2	2.47	0.44
1:B:541:ILE:HD13	1:B:570:LEU:CD2	2.47	0.44
1:A:608:ILE:HG13	1:A:663:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.65	0.44
1:B:561:GLN:O	1:B:562:GLU:C	2.60	0.44
1:C:94:MET:HE2	1:C:105:ILE:HG21	1.99	0.44
1:D:197:ILE:HG22	1:D:437:VAL:HG21	1.99	0.44
1:D:5:LEU:HD12	6:D:987:HOH:O	2.17	0.44
1:D:13:LEU:HD11	1:D:147:ILE:HD11	2.00	0.44
3:B:1801:B12:N23	4:D:1500:5AD:C4'	2.75	0.44
1:D:701:GLY:HA2	1:D:719:PHE:O	2.18	0.44
1:A:735:LYS:O	1:A:738:GLU:N	2.49	0.44
1:B:688:VAL:C	1:B:690:LYS:H	2.26	0.44
3:B:1801:B12:H261	4:D:1500:5AD:H5'3	2.00	0.44
3:C:1801:B12:H253	3:C:1801:B12:H301	1.81	0.44
2:H:57:MET:HE1	2:H:82:GLY:HA2	2.00	0.44
1:A:153:ARG:HA	1:A:154:PRO:HD3	1.90	0.44
1:A:613:VAL:HG22	1:A:614:GLY:H	1.82	0.44
1:A:668:THR:HB	1:A:676:HIS:HB2	1.99	0.44
5:A:767:Z98:H4A	1:C:629:LYS:HE3	1.87	0.44
1:C:13:LEU:HD22	1:C:18:ILE:CD1	2.47	0.44
1:D:600:ASP:OD2	1:D:600:ASP:C	2.61	0.44
2:H:40:LEU:HA	2:H:40:LEU:HD23	1.72	0.44
1:A:320:LEU:HD13	1:A:358:ALA:HB3	1.99	0.44
1:A:606:LEU:CD2	1:A:732:LEU:HD13	2.39	0.44
1:B:292:GLU:HG3	6:B:944:HOH:O	2.18	0.44
3:B:1801:B12:H473	3:B:1801:B12:C49	2.33	0.44
1:D:668:THR:HG23	1:D:668:THR:O	2.17	0.44
3:D:1801:B12:H203	3:D:1801:B12:H301	2.00	0.44
1:A:568:ILE:CG2	1:A:570:LEU:HD11	2.48	0.43
1:C:177:GLY:O	1:C:178:VAL:C	2.61	0.43
1:C:597:ILE:HD13	1:C:726:ILE:CD1	2.47	0.43
1:D:611:ALA:HB2	1:D:643:LEU:HB2	2.00	0.43
1:C:413:SER:OG	1:C:422:ASP:OD2	2.32	0.43
1:C:460:TYR:O	1:C:461:ASP:HB2	2.17	0.43
1:D:667:SER:OG	1:D:669:ILE:HD11	2.18	0.43
1:B:377:LEU:HB2	1:D:368:MET:HG2	2.00	0.43
1:D:648:PRO:O	1:D:649:VAL:C	2.60	0.43
1:B:79:THR:HB	1:B:332:SER:HA	2.00	0.43
1:C:13:LEU:CD1	1:C:91:ILE:HG22	2.48	0.43
1:A:369:VAL:CG1	1:C:369:VAL:HG13	2.48	0.43
1:A:542:GLU:HG3	1:C:583:LEU:HD23	2.01	0.43
1:B:687:ALA:HB3	1:B:693:ARG:HD3	2.00	0.43
1:D:196:MET:SD	1:D:402:PHE:CD1	3.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ARG:CZ	1:D:432:ILE:HD12	2.49	0.43
1:C:268:PRO:HA	1:C:269:PRO:HD3	1.83	0.43
1:D:428:ILE:HB	6:D:882:HOH:O	2.18	0.43
1:A:160:TYR:CE1	5:A:767:Z98:HG	2.53	0.43
1:A:484:VAL:HG12	1:A:486:ILE:CD1	2.49	0.43
3:B:1801:B12:C6	4:D:1500:5AD:H5'1	2.48	0.43
1:C:574:VAL:HG13	1:C:576:PHE:CE1	2.54	0.43
1:A:713:GLN:HA	1:A:713:GLN:NE2	2.34	0.43
1:A:184:ASP:HA	1:A:185:PRO:HD2	1.90	0.43
1:A:188:ASN:HB3	1:A:194:ILE:HB	2.01	0.43
1:B:658:GLU:HG2	6:B:966:HOH:O	2.17	0.43
1:C:270:THR:HG21	1:C:279:LEU:HD13	2.01	0.43
1:D:250:ILE:HG23	2:H:34:VAL:HG21	2.01	0.43
1:A:135:LYS:NZ	1:A:488:GLU:OE2	2.30	0.43
1:A:580:ILE:HD12	1:C:535:VAL:HG11	2.00	0.43
1:B:730:THR:HG22	1:B:734:LYS:HD2	2.01	0.43
1:D:116:TYR:HE2	1:D:120:ILE:HD13	1.84	0.43
1:D:281:LEU:HB3	1:D:282:PRO:HD3	2.00	0.43
1:D:528:PHE:CD2	1:D:528:PHE:C	2.96	0.43
1:A:422:ASP:OD1	1:A:422:ASP:N	2.51	0.42
1:B:161:VAL:O	1:B:161:VAL:CG1	2.67	0.42
1:C:631:GLY:O	1:C:725:GLY:HA3	2.19	0.42
1:A:344:TRP:CG	1:A:515:VAL:HB	2.54	0.42
1:B:301:ASN:O	1:B:305:MET:HE1	2.18	0.42
1:A:512:LYS:HB2	1:A:513:PRO:HD2	2.00	0.42
1:A:717:ALA:HB2	1:A:731:PHE:CE1	2.54	0.42
3:A:1801:B12:C36	3:A:1801:B12:C35	2.84	0.42
1:B:172:MET:HE1	1:B:173:PHE:HD1	1.84	0.42
1:B:322:ILE:HD13	1:B:322:ILE:HA	1.87	0.42
1:D:172:MET:HE2	1:D:173:PHE:HD1	1.84	0.42
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.75	0.42
1:B:587:PRO:C	6:B:848:HOH:O	2.61	0.42
1:C:5:LEU:O	1:C:5:LEU:HD23	2.19	0.42
1:C:668:THR:CG2	1:C:668:THR:O	2.68	0.42
1:D:680:MET:HE1	1:D:705:VAL:CG1	2.50	0.42
1:B:604:THR:O	1:B:736:ARG:NH2	2.37	0.42
1:C:551:GLU:CD	1:C:573:ARG:HE	2.28	0.42
2:G:89:ALA:HB2	2:G:99:ALA:HB2	2.01	0.42
1:D:424:ILE:HG21	1:D:426:ARG:CZ	2.50	0.42
1:A:445:MET:CE	1:A:447:PRO:CA	2.96	0.42
3:A:1801:B12:H473	3:A:1801:B12:H481	0.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:VAL:CG1	1:B:686:LEU:HD12	2.50	0.42
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.98	0.42
3:C:1801:B12:H473	3:C:1801:B12:H481	1.52	0.42
1:D:210:MET:HE3	1:D:215:MET:CE	2.49	0.42
1:D:649:VAL:CG1	1:D:683:ILE:HG13	2.49	0.42
1:A:541:ILE:O	1:A:545:LYS:HG2	2.20	0.42
1:B:517:TRP:O	1:B:518:GLN:C	2.60	0.42
1:C:79:THR:HB	6:C:790:HOH:O	2.19	0.42
1:C:626:ILE:HD13	1:C:640:VAL:HG11	2.00	0.42
2:F:25:ARG:O	2:F:29:MET:HG2	2.20	0.42
1:A:711:VAL:HA	1:A:715:VAL:O	2.20	0.42
5:A:767:Z98:C4A	1:C:629:LYS:HZ3	2.23	0.42
1:B:22:LEU:HB2	6:B:864:HOH:O	2.18	0.42
1:C:6:GLN:CG	1:C:7:LEU:N	2.80	0.42
1:D:268:PRO:HA	1:D:269:PRO:HD3	1.74	0.42
1:A:19:LEU:HD11	1:A:499:MET:HE2	2.02	0.42
3:A:1801:B12:H252	3:A:1801:B12:H601	2.02	0.42
1:C:504:GLU:C	1:C:506:ARG:H	2.27	0.42
1:D:95:ARG:O	1:D:98:ALA:HB3	2.20	0.42
1:D:475:CYS:HB2	2:H:56:ARG:O	2.20	0.42
1:D:668:THR:O	1:D:668:THR:HG22	2.18	0.42
3:D:1801:B12:H492	3:D:1801:B12:H471	2.01	0.42
1:A:515:VAL:HG23	1:A:516:GLU:HG2	2.02	0.41
1:A:688:VAL:HG22	1:A:693:ARG:HG2	2.02	0.41
1:B:282:PRO:HG3	1:B:377:LEU:CD1	2.50	0.41
1:B:513:PRO:O	1:B:521:GLY:CA	2.68	0.41
3:B:1801:B12:HM51	3:B:1801:B12:HM63	1.87	0.41
1:C:443:ASP:O	2:G:83:HIS:CE1	2.73	0.41
1:D:264:LEU:HD13	1:D:296:MET:HE2	2.01	0.41
1:D:266:THR:HG23	6:D:777:HOH:O	2.20	0.41
1:A:123:THR:HG23	1:A:135:LYS:HD3	2.03	0.41
1:A:724:LYS:HB2	1:A:726:ILE:HG22	2.01	0.41
1:C:109:ARG:NH2	1:C:114:SER:OG	2.54	0.41
1:C:577:SER:O	1:C:578:ILE:HD12	2.20	0.41
1:D:606:LEU:HD12	1:D:608:ILE:CD1	2.50	0.41
1:A:161:VAL:HG23	1:A:181:ALA:HB1	2.02	0.41
1:D:335:THR:O	1:D:338:GLU:HB2	2.21	0.41
1:D:578:ILE:HD13	1:D:578:ILE:HA	1.78	0.41
1:A:137:VAL:HG11	1:A:172:MET:HE1	2.01	0.41
1:B:5:LEU:HD23	1:B:5:LEU:C	2.44	0.41
1:B:123:THR:OG1	1:B:488:GLU:OE2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:THR:HB	1:B:645:THR:HG22	2.03	0.41
1:C:185:PRO:HB3	1:C:203:ALA:HB2	2.02	0.41
1:C:200:PHE:CD2	2:G:37:LEU:HD13	2.55	0.41
3:C:1801:B12:O7R	3:C:1801:B12:C2B	2.68	0.41
1:D:301:ASN:HB2	6:D:926:HOH:O	2.19	0.41
1:A:445:MET:HE2	1:A:446:ALA:C	2.46	0.41
1:C:122:GLY:HA2	1:C:487:ASP:O	2.20	0.41
1:C:617:GLU:HB2	3:C:1801:B12:C43	2.51	0.41
1:C:657:ILE:CG1	1:C:692:ILE:HD13	2.51	0.41
1:D:736:ARG:HD2	6:D:849:HOH:O	2.17	0.41
1:A:568:ILE:HG22	1:A:570:LEU:HD11	2.00	0.41
1:B:458:LYS:C	1:B:460:TYR:N	2.77	0.41
3:B:1801:B12:H492	3:B:1801:B12:H471	2.01	0.41
1:C:82:ILE:CG2	1:C:90:ASP:HB3	2.51	0.41
1:C:344:TRP:CD1	1:C:515:VAL:HB	2.56	0.41
1:C:445:MET:HE2	1:C:447:PRO:N	2.30	0.41
2:G:76:LEU:HB3	2:G:84:ILE:HD11	2.02	0.41
1:A:164:VAL:CG1	1:A:194:ILE:HG12	2.50	0.41
1:A:608:ILE:HD13	1:A:638:VAL:HG13	2.03	0.41
1:B:279:LEU:HD11	1:D:46:PHE:CE1	2.55	0.41
1:B:663:ALA:HA	1:B:697:MET:O	2.21	0.41
2:G:16:ASN:HD22	2:G:16:ASN:HA	1.73	0.41
1:D:233:GLU:HG2	1:D:235:TRP:CH2	2.56	0.41
1:A:349:ILE:N	1:A:349:ILE:CD1	2.84	0.41
1:A:371:LEU:HD23	1:C:369:VAL:HG22	2.03	0.41
1:A:389:VAL:HG13	2:E:29:MET:HE1	2.03	0.41
1:B:201:ILE:HD13	1:B:437:VAL:CG1	2.51	0.41
1:B:679:ASN:O	1:B:683:ILE:HD13	2.20	0.41
1:D:26:THR:HG22	1:D:27:PRO:CD	2.49	0.41
1:D:428:ILE:HG23	6:D:873:HOH:O	2.21	0.41
1:B:610:ALA:HA	1:B:665:LEU:O	2.21	0.40
1:A:618:HIS:CD2	3:A:1801:B12:H482	2.57	0.40
3:B:1801:B12:H473	3:B:1801:B12:H481	1.86	0.40
1:C:197:ILE:HG22	1:C:201:ILE:HD11	2.03	0.40
1:C:335:THR:HA	1:C:336:PRO:HD3	1.91	0.40
1:D:608:ILE:CG1	1:D:663:ALA:HB3	2.50	0.40
1:D:693:ARG:HH22	1:D:716:ASP:CG	2.29	0.40
1:D:495:VAL:O	1:D:499:MET:HG2	2.21	0.40
1:A:266:THR:HG23	1:A:266:THR:O	2.22	0.40
1:A:613:VAL:CG2	1:A:649:VAL:HG23	2.51	0.40
1:B:552:VAL:CG1	1:B:570:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:VAL:HG12	1:B:689:GLU:N	2.35	0.40
1:D:186:GLN:O	1:D:187:TYR:C	2.64	0.40
1:A:224:ALA:HB3	1:A:245:HIS:CE1	2.57	0.40
1:B:238:MET:SD	1:B:283:TYR:HB2	2.62	0.40
1:C:259:LYS:HA	1:C:262:ILE:HD12	2.02	0.40
1:D:138:ARG:HE	1:D:176:GLU:CD	2.30	0.40
1:D:185:PRO:O	1:D:189:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/763 (95%)	674 (93%)	42 (6%)	6 (1%)	16	25
1	B	722/763 (95%)	683 (95%)	32 (4%)	7 (1%)	12	20
1	C	722/763 (95%)	691 (96%)	22 (3%)	9 (1%)	10	16
1	D	722/763 (95%)	690 (96%)	30 (4%)	2 (0%)	36	50
2	E	107/121 (88%)	101 (94%)	5 (5%)	1 (1%)	14	22
2	F	107/121 (88%)	103 (96%)	3 (3%)	1 (1%)	14	22
2	G	107/121 (88%)	105 (98%)	2 (2%)	0	100	100
2	H	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
All	All	3316/3536 (94%)	3153 (95%)	137 (4%)	26 (1%)	16	25

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	462	GLU
1	B	7	LEU

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Mol	Chain	Res	Type
1	B	739	MET
1	C	6	GLN
1	C	505	PHE
2	E	93	ASN
1	B	6	GLN
1	B	689	GLU
1	C	461	ASP
1	B	69	ASP
1	C	582	SER
1	A	487	ASP
1	A	736	ARG
1	C	480	PRO
1	C	487	ASP
1	A	7	LEU
2	F	15	ALA
1	C	7	LEU
1	B	16	GLU
1	C	688	VAL
1	D	461	ASP
1	B	411	VAL
1	C	411	VAL
1	D	411	VAL
1	A	411	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/644 (93%)	559 (94%)	39 (6%)	15	27
1	B	604/644 (94%)	574 (95%)	30 (5%)	22	38
1	C	600/644 (93%)	565 (94%)	35 (6%)	18	32
1	D	602/644 (94%)	556 (92%)	46 (8%)	12	21
2	E	89/100 (89%)	82 (92%)	7 (8%)	11	19
2	F	90/100 (90%)	85 (94%)	5 (6%)	19	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	89/100 (89%)	82 (92%)	7 (8%)	11	19
2	H	89/100 (89%)	84 (94%)	5 (6%)	19	33
All	All	2761/2976 (93%)	2587 (94%)	174 (6%)	16	29

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	LEU
1	A	9	VAL
1	A	18	ILE
1	A	24	LYS
1	A	28	LYS
1	A	69	ASP
1	A	153	ARG
1	A	172	MET
1	A	232	ARG
1	A	250	ILE
1	A	306	GLU
1	A	341	ASN
1	A	349	ILE
1	A	411	VAL
1	A	418	GLU
1	A	449	THR
1	A	471	LEU
1	A	506	ARG
1	A	518	GLN
1	A	533	LYS
1	A	541	ILE
1	A	546	LYS
1	A	573	ARG
1	A	574	VAL
1	A	578	ILE
1	A	580	ILE
1	A	604	THR
1	A	608	ILE
1	A	651	LYS
1	A	668	THR
1	A	670	ILE
1	A	689	GLU
1	A	694	ASP

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Mol	Chain	Res	Type
1	A	696	ILE
1	A	706	THR
1	A	712	LYS
1	A	721	ARG
1	A	738	GLU
2	E	20	GLU
2	E	42	LYS
2	E	73	ASP
2	E	76	LEU
2	E	79	LYS
2	E	93	ASN
2	E	114	GLN
1	B	6	GLN
1	B	15	VAL
1	B	18	ILE
1	B	125	GLN
1	B	172	MET
1	B	232	ARG
1	B	292	GLU
1	B	306	GLU
1	B	338	GLU
1	B	341	ASN
1	B	349	ILE
1	B	411	VAL
1	B	428	ILE
1	B	442	GLU
1	B	457	VAL
1	B	464	LEU
1	B	471	LEU
1	B	557	ARG
1	B	578	ILE
1	B	580	ILE
1	B	592	LEU
1	B	603	LYS
1	B	608	ILE
1	B	613	VAL
1	B	651	LYS
1	B	668	THR
1	B	696	ILE
1	B	703	THR
1	B	723	SER
1	B	736	ARG

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Mol	Chain	Res	Type
2	F	20	GLU
2	F	31	GLU
2	F	76	LEU
2	F	92	LYS
2	F	101	LEU
1	C	7	LEU
1	C	9	VAL
1	C	13	LEU
1	C	20	LYS
1	C	26	THR
1	C	39	GLU
1	C	79	THR
1	C	164	VAL
1	C	168	ASP
1	C	232	ARG
1	C	301	ASN
1	C	306	GLU
1	C	341	ASN
1	C	411	VAL
1	C	428	ILE
1	C	462	GLU
1	C	464	LEU
1	C	465	VAL
1	C	471	LEU
1	C	500	GLU
1	C	570	LEU
1	C	576	PHE
1	C	578	ILE
1	C	604	THR
1	C	608	ILE
1	C	613	VAL
1	C	643	LEU
1	C	651	LYS
1	C	668	THR
1	C	683	ILE
1	C	694	ASP
1	C	696	ILE
1	C	731	PHE
1	C	733	VAL
1	C	736	ARG
2	G	8	GLN
2	G	9	GLN

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Mol	Chain	Res	Type
2	G	39	ASP
2	G	76	LEU
2	G	84	ILE
2	G	101	LEU
2	G	107	LYS
1	D	5	LEU
1	D	6	GLN
1	D	8	ARG
1	D	15	VAL
1	D	24	LYS
1	D	26	THR
1	D	28	LYS
1	D	39	GLU
1	D	47	ILE
1	D	127	ILE
1	D	153	ARG
1	D	172	MET
1	D	232	ARG
1	D	258	LYS
1	D	306	GLU
1	D	338	GLU
1	D	349	ILE
1	D	395	ILE
1	D	411	VAL
1	D	427	GLN
1	D	449	THR
1	D	471	LEU
1	D	491	GLU
1	D	546	LYS
1	D	557	ARG
1	D	577	SER
1	D	578	ILE
1	D	591	ILE
1	D	597	ILE
1	D	604	THR
1	D	606	LEU
1	D	608	ILE
1	D	613	VAL
1	D	615	GLU
1	D	635	LYS
1	D	657	ILE
1	D	659	LEU

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Mol	Chain	Res	Type
1	D	660	LYS
1	D	662	ASP
1	D	668	THR
1	D	669	ILE
1	D	682	ARG
1	D	683	ILE
1	D	694	ASP
1	D	696	ILE
1	D	736	ARG
2	H	24	THR
2	H	76	LEU
2	H	84	ILE
2	H	93	ASN
2	H	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	319	ASN
1	A	331	GLN
1	A	348	ASN
1	A	370	GLN
1	A	407	GLN
1	A	704	GLN
1	A	713	GLN
2	E	8	GLN
2	E	16	ASN
2	E	114	GLN
1	B	36	GLN
1	B	73	GLN
1	B	125	GLN
1	B	217	GLN
1	B	319	ASN
1	B	348	ASN
1	B	370	GLN
1	B	420	ASN
1	B	518	GLN
2	F	8	GLN
1	C	6	GLN
1	C	36	GLN
1	C	217	GLN

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Mol	Chain	Res	Type
1	C	301	ASN
1	C	357	GLN
1	C	370	GLN
1	C	518	GLN
2	G	8	GLN
2	G	16	ASN
2	G	93	ASN
1	D	6	GLN
1	D	36	GLN
1	D	228	ASN
1	D	319	ASN
1	D	341	ASN
1	D	370	GLN
1	D	403	ASN
2	H	16	ASN
2	H	83	HIS
2	H	93	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5AD	C	1500	3	20,20,20	1.74	3 (15%)	28,30,30	2.75	13 (46%)
3	B12	A	1801	1,4	94,101,101	1.47	11 (11%)	149,166,166	2.49	39 (26%)
3	B12	C	1801	1,4	94,101,101	1.75	13 (13%)	149,166,166	2.56	37 (24%)
5	Z98	D	767	-	22,23,23	1.53	3 (13%)	27,32,32	1.61	4 (14%)
4	5AD	D	1500	3	20,20,20	1.72	4 (20%)	28,30,30	3.14	13 (46%)
3	B12	D	1801	1,4	94,101,101	1.48	12 (12%)	149,166,166	2.39	36 (24%)
5	Z98	C	767	-	22,23,23	1.55	2 (9%)	27,32,32	1.73	6 (22%)
4	5AD	B	1500	3	20,20,20	1.73	4 (20%)	28,30,30	2.55	12 (42%)
5	Z98	B	767	-	22,23,23	1.55	6 (27%)	27,32,32	1.82	7 (25%)
3	B12	B	1801	1,4	94,101,101	1.77	11 (11%)	149,166,166	2.41	34 (22%)
4	5AD	A	1500	3	20,20,20	1.80	5 (25%)	28,30,30	2.85	15 (53%)
5	Z98	A	767	-	22,23,23	1.96	8 (36%)	27,32,32	2.32	5 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5AD	C	1500	3	-	0/4/20/20	0/3/3/3
3	B12	A	1801	1,4	1/1/36/38	18/56/223/223	0/3/11/11
3	B12	C	1801	1,4	1/1/36/38	10/56/223/223	0/3/11/11
5	Z98	D	767	-	-	8/17/17/17	0/1/1/1
4	5AD	D	1500	3	1/1/4/4	0/4/20/20	0/3/3/3
3	B12	D	1801	1,4	-	6/56/223/223	0/3/11/11
5	Z98	C	767	-	-	7/17/17/17	0/1/1/1
4	5AD	B	1500	3	-	0/4/20/20	0/3/3/3
5	Z98	B	767	-	-	7/17/17/17	0/1/1/1
3	B12	B	1801	1,4	1/1/36/38	7/56/223/223	0/3/11/11
4	5AD	A	1500	3	1/1/4/4	0/4/20/20	0/3/3/3
5	Z98	A	767	-	-	10/17/17/17	0/1/1/1

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C19-N24	-9.96	1.36	1.49
3	B	1801	B12	C19-N24	-9.45	1.37	1.49
3	B	1801	B12	C14-N23	6.99	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C14-N23	6.71	1.44	1.35
3	A	1801	B12	C14-N23	5.93	1.43	1.35
3	D	1801	B12	C14-N23	5.90	1.42	1.35
3	B	1801	B12	C8B-C9B	5.86	1.49	1.40
3	A	1801	B12	C19-N24	-5.84	1.41	1.49
4	C	1500	5AD	C5-C4	5.29	1.48	1.39
3	D	1801	B12	C8B-C9B	5.18	1.48	1.40
3	D	1801	B12	C19-N24	-5.08	1.42	1.49
4	A	1500	5AD	C5-C4	4.90	1.47	1.39
4	B	1500	5AD	C5-C4	4.85	1.47	1.39
4	D	1500	5AD	C5-C4	4.37	1.46	1.39
3	C	1801	B12	C9-N22	4.17	1.40	1.30
5	C	767	Z98	P-OP2	4.11	1.63	1.50
3	A	1801	B12	C8B-C9B	4.09	1.47	1.40
3	B	1801	B12	C9-N22	4.08	1.40	1.30
5	A	767	Z98	P-OP2	3.78	1.62	1.50
5	A	767	Z98	OP4-C5A	-3.73	1.31	1.44
4	D	1500	5AD	C5-C6	3.71	1.51	1.41
3	C	1801	B12	C8B-C9B	3.59	1.46	1.40
5	A	767	Z98	C2A-C2	3.57	1.56	1.50
3	D	1801	B12	C11-N23	3.47	1.43	1.36
3	D	1801	B12	C9-N22	3.46	1.39	1.30
3	C	1801	B12	C16-C15	-3.46	1.34	1.44
3	B	1801	B12	C16-C15	-3.44	1.34	1.44
3	D	1801	B12	C16-C15	-3.34	1.35	1.44
3	A	1801	B12	C8B-N1B	-3.32	1.32	1.39
3	D	1801	B12	C6B-C5B	3.30	1.48	1.40
4	C	1500	5AD	C5-C6	3.27	1.50	1.41
3	A	1801	B12	C6B-C5B	3.27	1.48	1.40
3	A	1801	B12	C16-C15	-3.19	1.35	1.44
3	A	1801	B12	C11-N23	3.15	1.42	1.36
3	A	1801	B12	C10-C9	3.14	1.48	1.39
3	B	1801	B12	C6B-C5B	3.14	1.48	1.40
5	A	767	Z98	C4-C4A	-3.14	1.40	1.46
3	B	1801	B12	C9B-N3B	-3.10	1.34	1.39
3	A	1801	B12	C9B-N3B	-3.06	1.34	1.39
3	A	1801	B12	C9-N22	3.04	1.38	1.30
4	B	1500	5AD	C5-C6	3.00	1.49	1.41
3	D	1801	B12	C10-C9	2.97	1.47	1.39
3	C	1801	B12	C11-N23	2.97	1.42	1.36
5	B	767	Z98	P-OP2	2.93	1.59	1.50
4	C	1500	5AD	C8-N7	2.93	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	767	Z98	C2A-C2	2.92	1.55	1.50
3	B	1801	B12	C2B-N3B	2.91	1.37	1.31
4	A	1500	5AD	C8-N7	2.90	1.37	1.31
3	C	1801	B12	C14-C15	2.82	1.50	1.38
3	D	1801	B12	C8B-N1B	-2.81	1.33	1.39
4	A	1500	5AD	C5-C6	2.75	1.48	1.41
3	D	1801	B12	C14-C15	2.74	1.50	1.38
5	B	767	Z98	C4-C4A	-2.73	1.40	1.46
3	C	1801	B12	C9B-N3B	-2.71	1.34	1.39
5	B	767	Z98	C3-C2	-2.71	1.38	1.41
5	B	767	Z98	C4A-ND	2.65	1.36	1.27
4	D	1500	5AD	C8-N7	2.64	1.36	1.31
3	A	1801	B12	C14-C15	2.59	1.49	1.38
5	A	767	Z98	P-OP3	2.57	1.64	1.54
3	B	1801	B12	C14-C15	2.48	1.49	1.38
5	D	767	Z98	C4A-ND	2.47	1.35	1.27
4	B	1500	5AD	C8-N7	2.45	1.36	1.31
3	C	1801	B12	C2B-N3B	2.42	1.36	1.31
3	B	1801	B12	C8B-N1B	-2.39	1.34	1.39
3	C	1801	B12	C12-C11	-2.39	1.48	1.52
4	A	1500	5AD	C5-N7	-2.38	1.34	1.39
3	B	1801	B12	C11-N23	2.38	1.41	1.36
3	D	1801	B12	C9B-N3B	-2.35	1.35	1.39
4	A	1500	5AD	C3'-C2'	-2.35	1.47	1.53
5	C	767	Z98	C4A-ND	2.31	1.34	1.27
3	C	1801	B12	C6B-C5B	2.31	1.46	1.40
5	B	767	Z98	C2A-C2	2.30	1.54	1.50
3	C	1801	B12	C10-C11	-2.28	1.30	1.37
5	A	767	Z98	P-OP1	-2.22	1.46	1.54
5	D	767	Z98	C4-C4A	-2.18	1.42	1.46
3	C	1801	B12	C2B-N1B	-2.11	1.34	1.37
4	B	1500	5AD	C4-N3	2.09	1.38	1.34
4	D	1500	5AD	O4'-C1'	2.08	1.46	1.42
5	A	767	Z98	C4-C5	-2.07	1.39	1.42
5	B	767	Z98	O-C	-2.05	1.24	1.30
3	D	1801	B12	C1-C2	-2.02	1.54	1.58
5	A	767	Z98	C4A-ND	2.01	1.33	1.27

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	B12	C20-C1-C19	-11.59	98.19	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C20-C1-C19	-10.08	99.64	109.35
3	A	1801	B12	C1-C19-N24	9.38	116.69	106.25
3	C	1801	B12	C20-C1-C19	-9.37	100.33	109.35
3	C	1801	B12	C12-C11-C10	-9.11	111.66	123.40
3	D	1801	B12	C1-C19-N24	9.07	116.34	106.25
3	A	1801	B12	C13-C12-C11	-8.91	91.01	100.97
3	D	1801	B12	C13-C12-C11	-8.25	91.75	100.97
3	C	1801	B12	C19-C1-N21	8.13	110.52	102.14
3	C	1801	B12	C47-C12-C46	8.10	122.83	109.41
3	C	1801	B12	C13-C12-C11	-8.04	91.98	100.97
3	D	1801	B12	C20-C1-C19	-7.93	101.72	109.35
3	B	1801	B12	C1-C19-N24	7.44	114.52	106.25
5	A	767	Z98	OP3-P-OP4	-7.32	87.60	106.67
3	A	1801	B12	C1-C19-C18	7.31	133.76	121.90
3	B	1801	B12	C19-C1-N21	7.29	109.65	102.14
3	D	1801	B12	C19-C1-N21	7.25	109.61	102.14
3	C	1801	B12	C1-C19-N24	7.22	114.28	106.25
4	D	1500	5AD	C5-C4-N3	-7.07	116.98	126.72
3	B	1801	B12	C13-C12-C11	-7.01	93.13	100.97
3	D	1801	B12	C12-C11-C10	-6.94	114.45	123.40
3	C	1801	B12	C18-C19-N24	6.90	112.70	102.33
5	A	767	Z98	OP1-P-OP4	6.77	124.33	106.67
3	B	1801	B12	C18-C19-N24	6.67	112.36	102.33
3	D	1801	B12	C46-C12-C13	-6.65	85.78	112.74
3	A	1801	B12	C19-C1-N21	6.52	108.86	102.14
3	B	1801	B12	C12-C11-C10	-6.52	114.99	123.40
3	A	1801	B12	C47-C12-C46	6.50	120.18	109.41
3	D	1801	B12	C1-C19-C18	6.46	132.38	121.90
3	A	1801	B12	C46-C12-C13	-6.45	86.59	112.74
4	D	1500	5AD	O2'-C2'-C1'	6.25	131.62	110.10
3	C	1801	B12	C20-C1-N21	-6.23	99.96	110.26
4	A	1500	5AD	C5-C4-N3	-6.23	118.14	126.72
4	C	1500	5AD	C5-C4-N3	-6.18	118.20	126.72
3	D	1801	B12	C47-C12-C46	6.15	119.59	109.41
4	B	1500	5AD	C5-C4-N3	-6.12	118.29	126.72
5	C	767	Z98	CG-ND-C4A	6.07	138.15	118.72
3	C	1801	B12	C12-C11-N23	5.81	119.84	111.83
3	B	1801	B12	C2-C1-C19	5.79	127.62	118.61
3	B	1801	B12	C1-C19-C18	5.60	130.98	121.90
3	C	1801	B12	C46-C12-C13	-5.55	90.25	112.74
3	C	1801	B12	C1-C19-C18	5.55	130.90	121.90
4	D	1500	5AD	C2-N3-C4	5.37	124.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C47-C12-C13	-5.37	90.97	112.74
3	B	1801	B12	C46-C12-C13	-5.33	91.13	112.74
3	A	1801	B12	C12-C11-C10	-5.32	116.55	123.40
4	B	1500	5AD	N3-C4-N9	5.31	136.19	127.17
3	D	1801	B12	C19-N24-C16	5.19	112.97	107.29
4	D	1500	5AD	C3'-C2'-C1'	5.18	111.25	101.46
3	B	1801	B12	C47-C12-C46	5.13	117.89	109.41
3	A	1801	B12	C9B-C8B-N1B	5.10	107.56	105.30
5	B	767	Z98	CG-ND-C4A	5.08	134.98	118.72
4	C	1500	5AD	N3-C4-N9	5.07	135.78	127.17
3	A	1801	B12	C12-C11-N23	5.05	118.78	111.83
4	A	1500	5AD	C3'-C2'-C1'	5.04	111.00	101.46
3	D	1801	B12	C12-C11-N23	5.03	118.75	111.83
3	A	1801	B12	C26-C2-C1	5.00	117.73	110.00
3	B	1801	B12	C12-C11-N23	4.91	118.59	111.83
4	A	1500	5AD	O2'-C2'-C1'	4.90	126.98	110.10
3	D	1801	B12	C25-C2-C1	-4.90	106.43	113.75
4	A	1500	5AD	N3-C4-N9	4.89	135.49	127.17
3	B	1801	B12	C9B-C8B-N1B	4.86	107.46	105.30
3	A	1801	B12	C2-C1-N21	4.75	108.38	101.78
4	D	1500	5AD	N3-C4-N9	4.75	135.24	127.17
4	D	1500	5AD	C4-C5-N7	-4.69	105.22	110.58
4	D	1500	5AD	N3-C2-N1	-4.66	121.53	128.58
3	C	1801	B12	C9-C10-C11	-4.64	119.34	125.97
3	A	1801	B12	C2-C1-C19	4.57	125.72	118.61
3	A	1801	B12	C20-C1-N21	-4.55	102.73	110.26
3	C	1801	B12	C2-C1-C19	4.44	125.52	118.61
4	C	1500	5AD	C2-N3-C4	4.38	122.53	111.83
3	A	1801	B12	C19-N24-C16	4.37	112.07	107.29
3	C	1801	B12	C9B-C8B-N1B	4.28	107.20	105.30
4	B	1500	5AD	N3-C2-N1	-4.26	122.13	128.58
4	B	1500	5AD	C2-N3-C4	4.23	122.16	111.83
3	C	1801	B12	C17-C16-C15	4.19	132.89	126.26
4	A	1500	5AD	C2-N3-C4	4.18	122.03	111.83
3	C	1801	B12	C8B-C9B-N3B	-4.17	105.49	110.00
3	D	1801	B12	C8B-C9B-N3B	-4.13	105.54	110.00
4	A	1500	5AD	N3-C2-N1	-4.12	122.34	128.58
3	D	1801	B12	C18-C19-N24	4.10	108.50	102.33
3	D	1801	B12	C9B-C8B-N1B	4.10	107.12	105.30
4	C	1500	5AD	C3'-C2'-C1'	4.08	109.17	101.46
3	D	1801	B12	C2-C1-N21	4.07	107.44	101.78
4	C	1500	5AD	N3-C2-N1	-4.04	122.47	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	767	Z98	OP1-P-OP4	4.02	117.16	106.67
3	B	1801	B12	C47-C12-C11	4.00	124.38	110.08
4	C	1500	5AD	O2'-C2'-C1'	3.98	123.82	110.10
3	C	1801	B12	C7B-C8B-C9B	-3.98	117.71	122.47
3	D	1801	B12	C17-C16-C15	3.97	132.54	126.26
3	B	1801	B12	C47-C12-C13	-3.94	96.75	112.74
3	B	1801	B12	C8B-C9B-N3B	-3.91	105.77	110.00
3	D	1801	B12	C47-C12-C13	-3.90	96.91	112.74
3	B	1801	B12	C9-C10-C11	-3.88	120.42	125.97
3	A	1801	B12	C8B-C9B-N3B	-3.87	105.82	110.00
3	A	1801	B12	C17-C16-C15	3.86	132.37	126.26
5	D	767	Z98	OP4-C5A-C5	3.82	116.52	109.36
3	B	1801	B12	C20-C1-C2	-3.80	107.01	113.28
4	C	1500	5AD	O2'-C2'-C3'	3.73	123.76	111.82
3	C	1801	B12	C9B-N3B-C2B	3.68	108.91	104.40
4	B	1500	5AD	O4'-C1'-N9	3.67	115.14	108.09
4	A	1500	5AD	O2'-C2'-C3'	-3.66	100.09	111.82
3	C	1801	B12	C47-C12-C13	-3.65	97.96	112.74
4	A	1500	5AD	C4-C5-N7	-3.64	106.42	110.58
4	D	1500	5AD	C5-N7-C8	3.59	109.10	103.45
3	A	1801	B12	C15-C14-N23	-3.59	121.94	126.26
3	C	1801	B12	C47-C12-C11	3.55	122.75	110.08
3	D	1801	B12	C20-C1-C2	-3.52	107.48	113.28
3	D	1801	B12	C12-C13-C14	3.51	108.03	102.26
3	A	1801	B12	C18-C19-N24	3.51	107.60	102.33
4	C	1500	5AD	C4-C5-N7	-3.50	106.58	110.58
3	B	1801	B12	C18-C17-C16	3.49	104.90	100.69
3	C	1801	B12	C15-C16-N24	-3.48	117.46	122.42
3	B	1801	B12	C17-C16-C15	3.44	131.70	126.26
3	D	1801	B12	C18-C17-C16	3.41	104.81	100.69
4	D	1500	5AD	C6-C5-N7	3.40	138.64	132.09
3	C	1801	B12	C12-C13-C14	3.39	107.83	102.26
3	D	1801	B12	C10-C9-N22	-3.33	121.95	125.74
3	C	1801	B12	C19-N24-C16	3.31	110.91	107.29
5	A	767	Z98	CG-ND-C4A	3.30	129.30	118.72
4	A	1500	5AD	C5-N7-C8	3.23	108.53	103.45
3	B	1801	B12	C54-C17-C18	-3.22	108.37	112.99
4	B	1500	5AD	C4-C5-N7	-3.22	106.91	110.58
4	B	1500	5AD	C4-N9-C8	3.19	109.09	105.74
3	A	1801	B12	C47-C12-C11	3.18	121.44	110.08
3	D	1801	B12	C9B-N3B-C2B	3.16	108.28	104.40
4	C	1500	5AD	C4-N9-C8	3.16	109.05	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1801	B12	C2-C1-C19	3.14	123.50	118.61
3	A	1801	B12	C54-C17-C18	-3.12	108.51	112.99
3	C	1801	B12	C18-C17-C16	3.11	104.44	100.69
3	A	1801	B12	C18-C17-C16	3.06	104.38	100.69
3	B	1801	B12	C19-N24-C16	3.03	110.60	107.29
4	B	1500	5AD	C5-N7-C8	2.99	108.16	103.45
3	A	1801	B12	C9B-N3B-C2B	2.99	108.07	104.40
3	C	1801	B12	C2-C1-N21	2.99	105.93	101.78
3	D	1801	B12	C4B-C9B-N3B	2.96	135.49	130.51
3	C	1801	B12	O6R-C4R-C5R	2.95	115.46	109.22
3	D	1801	B12	C47-C12-C11	2.94	120.58	110.08
4	C	1500	5AD	C5-N7-C8	2.94	108.06	103.45
5	C	767	Z98	C4-C4A-ND	-2.90	110.66	124.04
3	B	1801	B12	C15-C16-N24	-2.88	118.33	122.42
3	C	1801	B12	C5R-C4R-C3R	-2.84	105.89	114.84
4	C	1500	5AD	C5'-C4'-C3'	-2.83	112.72	115.70
3	A	1801	B12	C12-C13-C14	2.83	106.91	102.26
3	B	1801	B12	C9B-N3B-C2B	2.81	107.84	104.40
3	B	1801	B12	C15-C14-N23	-2.80	122.88	126.26
3	C	1801	B12	C26-C2-C1	2.79	114.32	110.00
4	D	1500	5AD	N9-C8-N7	-2.77	110.01	113.94
3	D	1801	B12	C20-C1-N21	-2.76	105.70	110.26
3	B	1801	B12	C7B-C8B-C9B	-2.74	119.19	122.47
5	B	767	Z98	OP3-P-OP2	-2.72	100.23	110.83
3	C	1801	B12	C3-C4-N21	-2.67	108.66	111.98
3	D	1801	B12	C46-C12-C11	2.67	119.63	110.08
5	D	767	Z98	CG-ND-C4A	2.66	127.25	118.72
3	A	1801	B12	C20-C1-C2	-2.62	108.96	113.28
3	D	1801	B12	C15-C16-N24	-2.61	118.70	122.42
3	A	1801	B12	O6R-C1R-N1B	2.60	113.08	108.09
4	A	1500	5AD	O3'-C3'-C4'	2.57	116.77	110.47
3	D	1801	B12	C8B-N1B-C1R	-2.57	121.06	125.41
3	B	1801	B12	C53-C15-C16	-2.57	116.01	120.36
4	C	1500	5AD	N9-C8-N7	-2.56	110.30	113.94
3	B	1801	B12	C48-C13-C12	2.54	123.80	116.52
3	D	1801	B12	C9-C10-C11	-2.54	122.34	125.97
3	B	1801	B12	C7-C6-C5	-2.54	124.10	128.07
4	B	1500	5AD	N9-C8-N7	-2.54	110.33	113.94
5	A	767	Z98	CB-CG-ND	2.53	117.50	110.82
3	C	1801	B12	O2-P-O4	-2.51	101.79	109.81
5	B	767	Z98	C3-C4-C4A	-2.49	115.91	120.40
4	C	1500	5AD	C6-C5-N7	2.48	136.87	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C7-C6-C5	-2.47	124.21	128.07
3	B	1801	B12	O3-C2P-C1P	2.47	111.83	106.94
4	A	1500	5AD	N9-C8-N7	-2.46	110.45	113.94
3	A	1801	B12	C25-C2-C1	-2.43	110.13	113.75
5	A	767	Z98	C2A-C2-C3	2.42	123.63	120.80
3	B	1801	B12	C36-C7-C37	2.42	114.85	110.74
4	D	1500	5AD	O4'-C1'-C2'	-2.41	101.45	106.62
3	D	1801	B12	C54-C17-C18	-2.41	109.53	112.99
4	D	1500	5AD	C5'-C4'-C3'	-2.40	113.18	115.70
4	B	1500	5AD	C6-C5-N7	2.36	136.64	132.09
4	A	1500	5AD	C6-C5-N7	2.36	136.63	132.09
4	A	1500	5AD	C4-N9-C8	2.35	108.21	105.74
3	B	1801	B12	C60-C18-C19	2.35	120.69	114.59
3	A	1801	B12	C15-C16-N24	-2.35	119.08	122.42
3	B	1801	B12	C2-C1-N21	2.34	105.03	101.78
3	D	1801	B12	C17-C16-N24	-2.33	107.61	111.17
4	A	1500	5AD	C5'-C4'-C3'	-2.33	113.26	115.70
3	A	1801	B12	C46-C12-C11	2.32	118.37	110.08
3	D	1801	B12	C15-C14-N23	-2.31	123.48	126.26
3	C	1801	B12	C2P-C1P-N59	-2.29	109.55	112.92
5	B	767	Z98	C4-C4A-ND	2.28	134.57	124.04
3	D	1801	B12	C7-C6-C5	-2.26	124.54	128.07
3	B	1801	B12	C12-C13-C14	2.25	105.96	102.26
3	A	1801	B12	C7-C6-N22	2.24	112.02	107.94
5	C	767	Z98	CB-CG-ND	-2.23	104.94	110.82
4	A	1500	5AD	C2'-C1'-N9	-2.22	107.78	113.30
3	B	1801	B12	C3-C4-N21	-2.22	109.22	111.98
4	B	1500	5AD	C2'-C1'-N9	-2.20	107.83	113.30
4	B	1500	5AD	C3'-C2'-C1'	2.20	105.62	101.46
3	D	1801	B12	C3R-C2R-C1R	2.19	104.70	99.89
3	C	1801	B12	N1B-C2B-N3B	-2.17	110.85	113.94
5	B	767	Z98	C2A-C2-N1	2.17	121.73	117.64
5	C	767	Z98	C2A-C2-C3	-2.16	118.27	120.80
3	A	1801	B12	C10-C9-N22	-2.14	123.30	125.74
3	D	1801	B12	C2P-C1P-N59	-2.14	109.78	112.92
5	C	767	Z98	C2A-C2-N1	2.12	121.64	117.64
5	D	767	Z98	C2A-C2-N1	2.12	121.63	117.64
3	C	1801	B12	C4B-C9B-N3B	2.11	134.06	130.51
5	C	767	Z98	CG-CB-CA	2.10	117.98	112.72
3	A	1801	B12	C37-C7-C8	2.08	113.86	108.37
5	B	767	Z98	C5-C4-C4A	2.08	124.68	121.47
3	A	1801	B12	C56-C55-C17	2.08	119.59	115.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C7B-C8B-C9B	-2.06	120.00	122.47
3	C	1801	B12	C10-C11-N23	2.05	127.88	124.42
3	C	1801	B12	C15-C14-N23	-2.03	123.81	126.26
3	A	1801	B12	C9-N22-C6	-2.03	102.83	105.28
3	C	1801	B12	O2-P-O3	2.03	108.54	102.87
4	D	1500	5AD	C4-N9-C8	2.03	107.87	105.74
3	A	1801	B12	C9-C10-C11	-2.02	123.08	125.97
5	B	767	Z98	C5A-C5-C6	-2.01	116.08	119.36
3	C	1801	B12	C3R-C2R-C1R	2.00	104.30	99.89
3	A	1801	B12	C26-C2-C3	-2.00	103.92	107.42

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1801	B12	C19
3	B	1801	B12	C19
3	C	1801	B12	C19
4	A	1500	5AD	C2'
4	D	1500	5AD	C2'

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C16-C17-C55-C56
3	A	1801	B12	C2R-C1R-N1B-C2B
5	A	767	Z98	C5A-OP4-P-OP1
5	A	767	Z98	C5A-OP4-P-OP2
5	A	767	Z98	C5A-OP4-P-OP3
5	A	767	Z98	N-CA-CB-CG
5	A	767	Z98	CA-CB-CG-ND
5	A	767	Z98	C4-C4A-ND-CG
5	B	767	Z98	N-CA-CB-CG
5	B	767	Z98	CA-CB-CG-ND
5	B	767	Z98	C4-C4A-ND-CG
5	C	767	Z98	C5-C4-C4A-ND
5	C	767	Z98	CA-CB-CG-ND
5	D	767	Z98	CA-CB-CG-ND
5	D	767	Z98	C4-C4A-ND-CG
3	C	1801	B12	C3R-C4R-C5R-O8R
3	C	1801	B12	C4-C3-C30-C31
3	C	1801	B12	O6R-C4R-C5R-O8R
3	B	1801	B12	C2R-C1R-N1B-C2B

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Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
3	B	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C16-C17-C55-C56
3	B	1801	B12	C2R-C1R-N1B-C8B
5	A	767	Z98	C5-C4-C4A-ND
3	A	1801	B12	N59-C1P-C2P-O3
3	C	1801	B12	C2R-C1R-N1B-C2B
5	A	767	Z98	C3-C4-C4A-ND
5	B	767	Z98	C3-C4-C4A-ND
3	C	1801	B12	C2-C3-C30-C31
3	A	1801	B12	O6R-C4R-C5R-O8R
3	A	1801	B12	C2-C3-C30-C31
5	C	767	Z98	C3-C4-C4A-ND
3	A	1801	B12	N59-C1P-C2P-C3P
3	A	1801	B12	C2R-C1R-N1B-C8B
3	C	1801	B12	C2R-C1R-N1B-C8B
5	B	767	Z98	C5-C4-C4A-ND
3	B	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C2R-C1R-N1B-C2B
5	B	767	Z98	OXT-C-CA-CB
3	A	1801	B12	C4-C3-C30-C31
3	B	1801	B12	O6R-C1R-N1B-C8B
3	C	1801	B12	O6R-C1R-N1B-C8B
5	C	767	Z98	C-CA-CB-CG
5	B	767	Z98	O-C-CA-CB
5	D	767	Z98	C3-C4-C4A-ND
5	D	767	Z98	N-CA-CB-CG
3	A	1801	B12	C42-C41-C8-C7
3	A	1801	B12	C3R-C4R-C5R-O8R
5	C	767	Z98	CB-CG-ND-C4A
3	A	1801	B12	C14-C13-C48-C49
3	A	1801	B12	C48-C49-C50-O51
3	A	1801	B12	O6R-C1R-N1B-C8B
3	D	1801	B12	C2R-C1R-N1B-C8B
3	D	1801	B12	O6R-C1R-N1B-C8B
5	A	767	Z98	O-C-CA-CB
5	A	767	Z98	OXT-C-CA-CB
5	C	767	Z98	OXT-C-CA-CB
5	C	767	Z98	O-C-CA-CB
5	D	767	Z98	O-C-CA-CB
5	D	767	Z98	OXT-C-CA-CB

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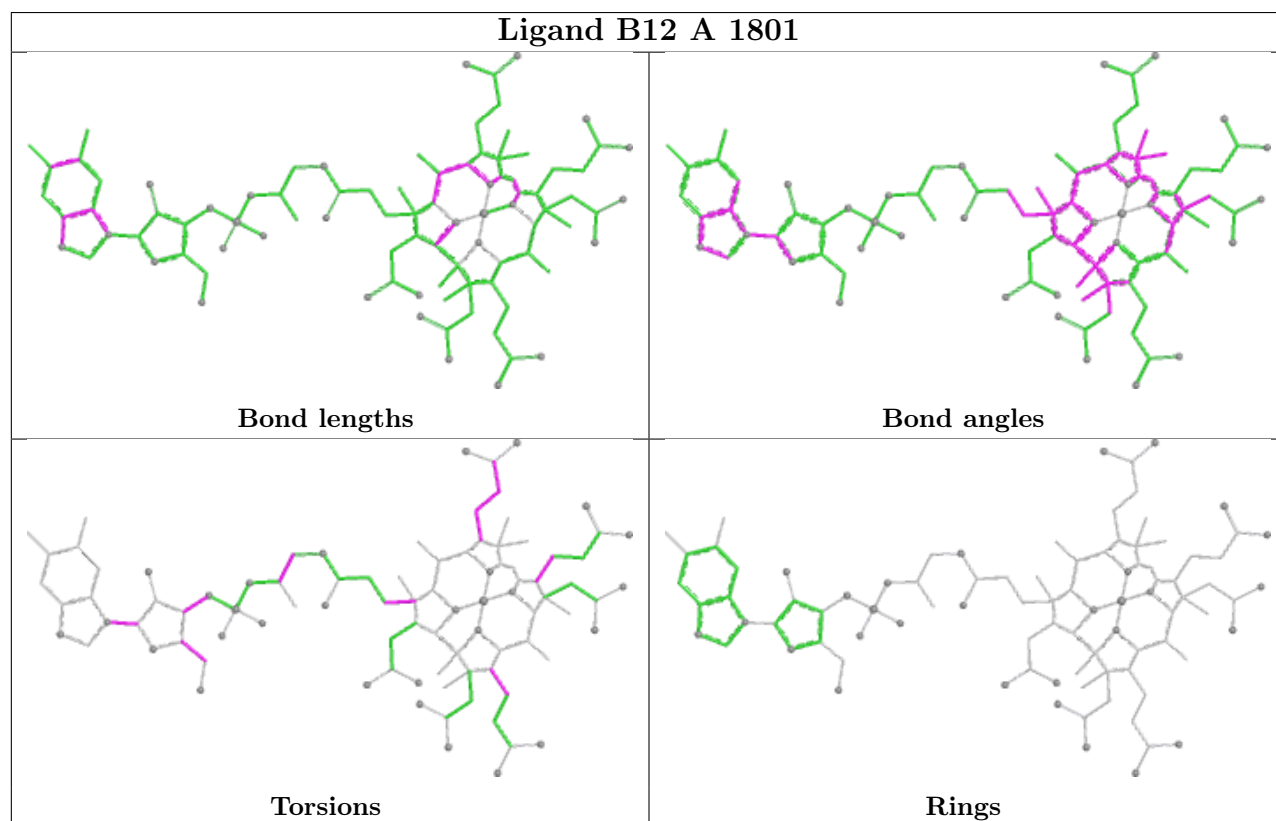
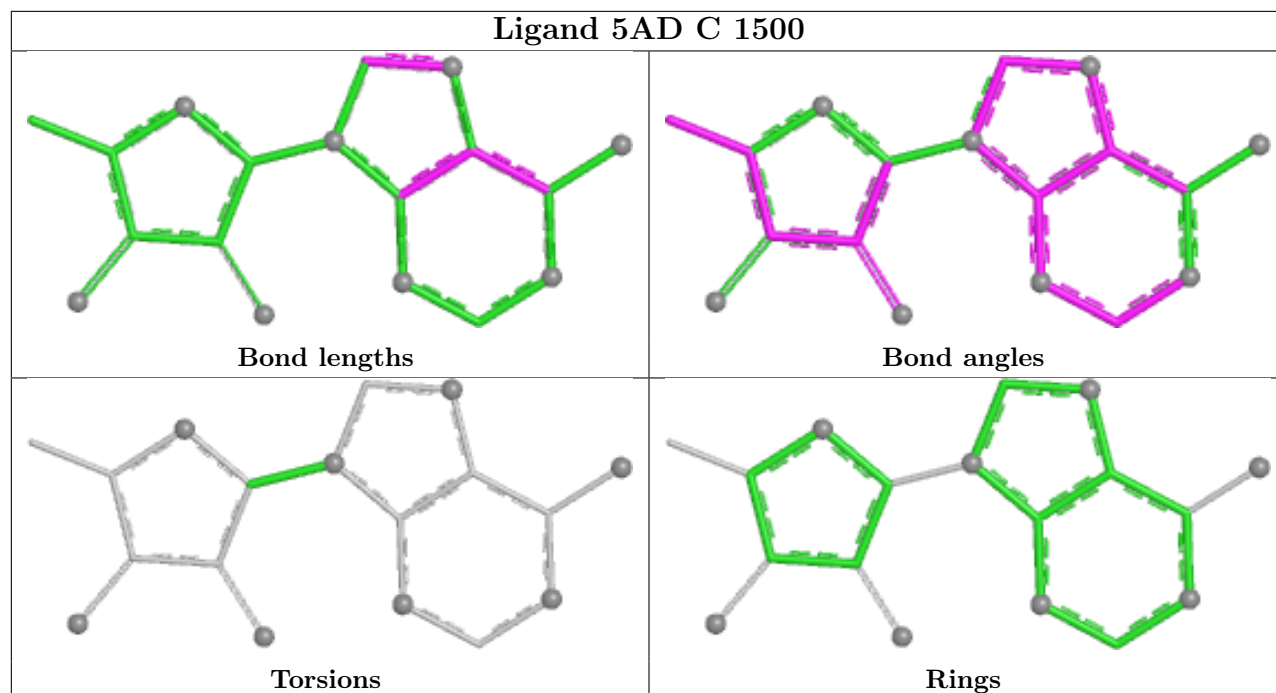
Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C13-C48-C49-C50
3	D	1801	B12	O6R-C1R-N1B-C2B
3	A	1801	B12	C12-C13-C48-C49
5	D	767	Z98	C5-C4-C4A-ND
3	A	1801	B12	C2R-C3R-O2-P
3	B	1801	B12	C2P-O3-P-O5
3	C	1801	B12	O6R-C1R-N1B-C2B
3	A	1801	B12	C42-C41-C8-C9
3	C	1801	B12	C55-C56-C57-O58
3	C	1801	B12	C55-C56-C57-N59
3	B	1801	B12	O6R-C1R-N1B-C2B
5	D	767	Z98	O-C-CA-N

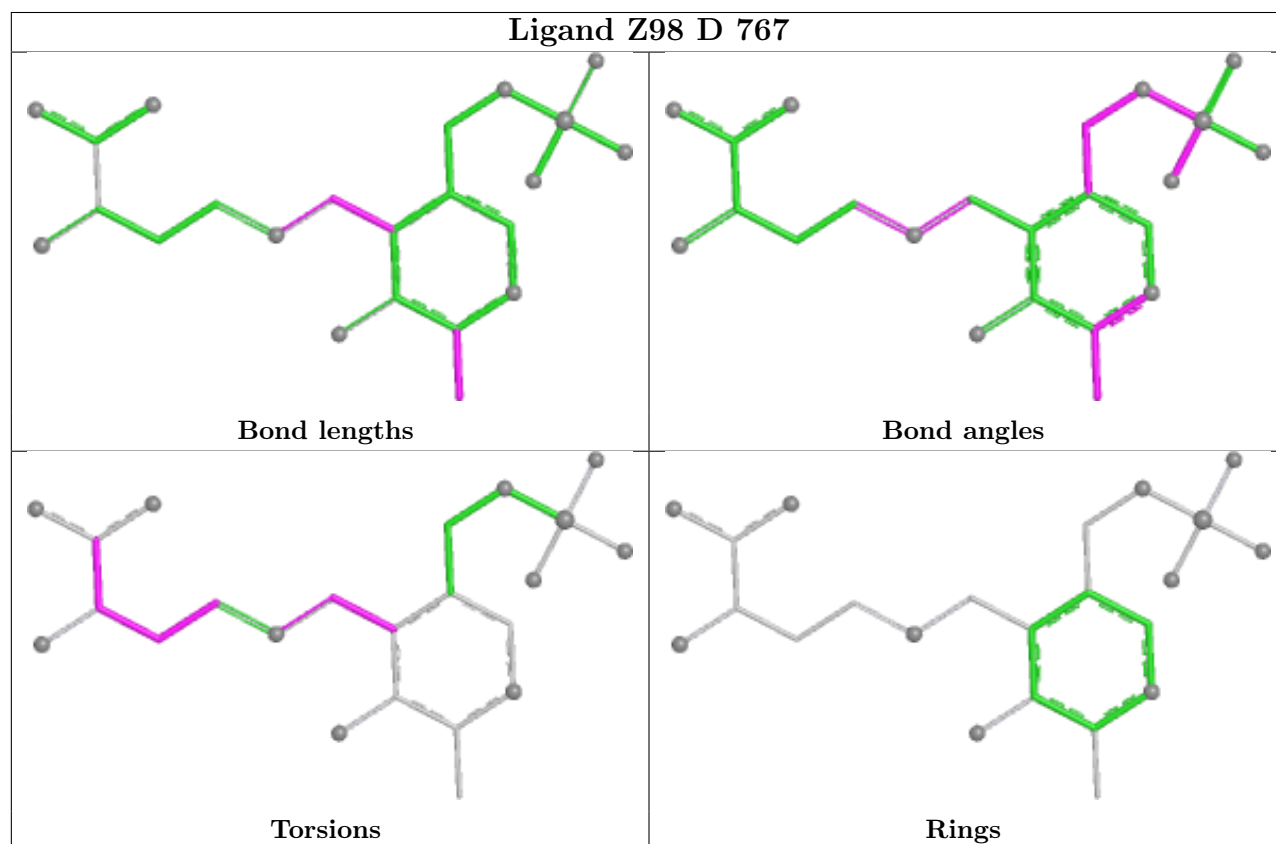
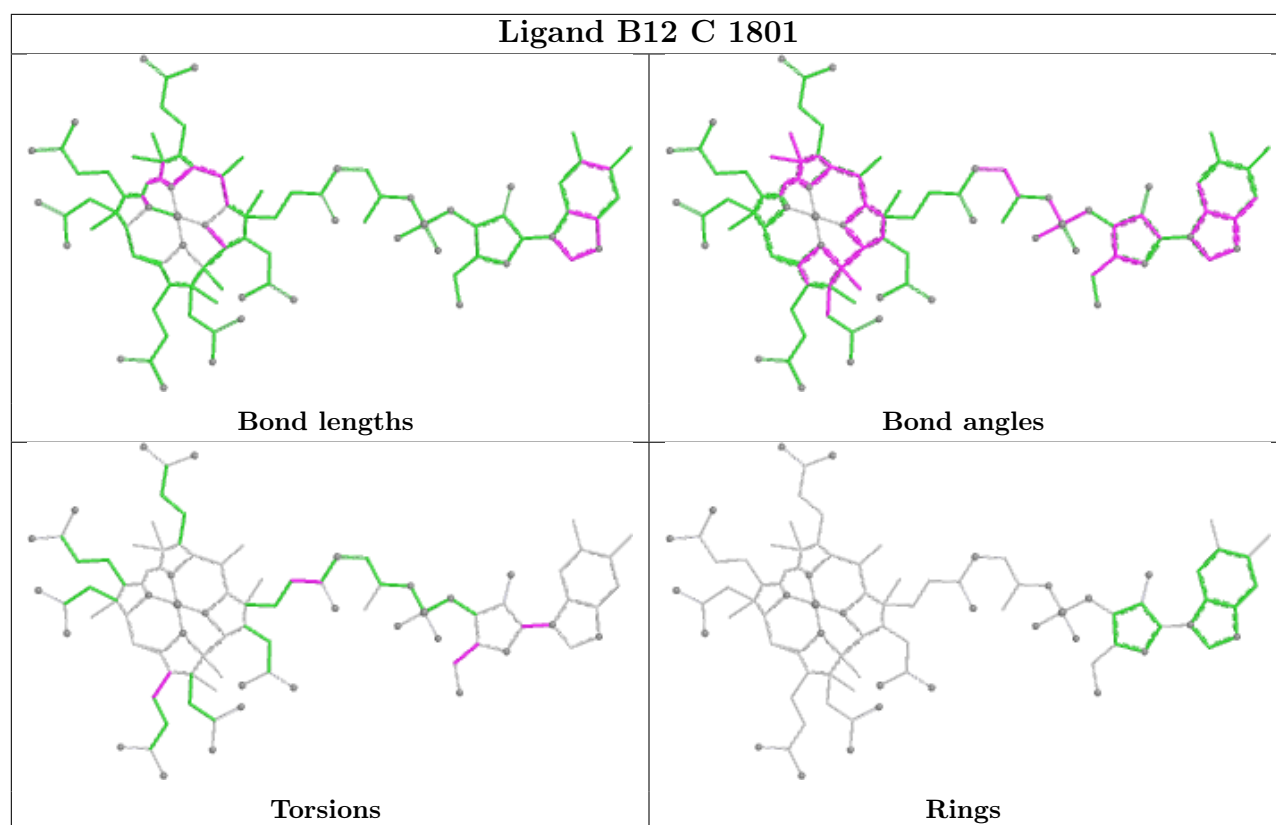
There are no ring outliers.

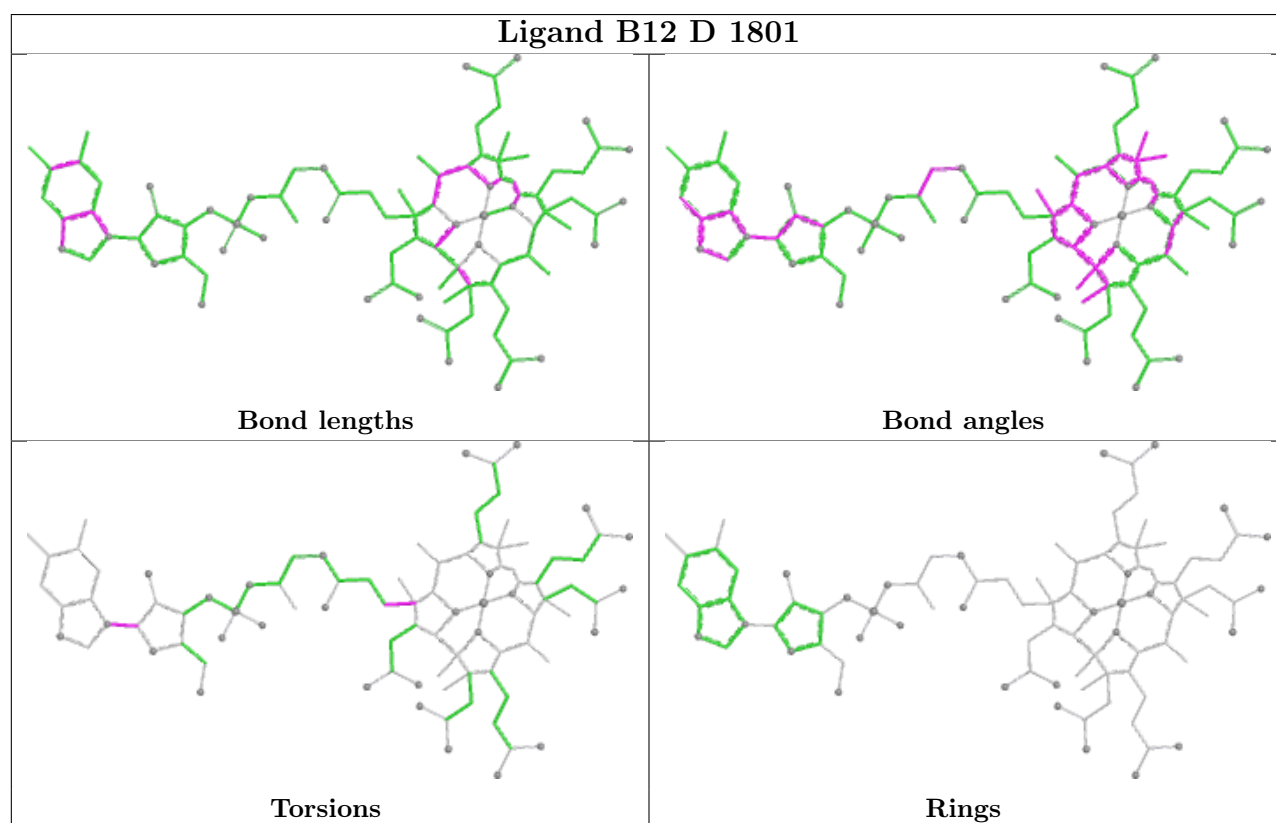
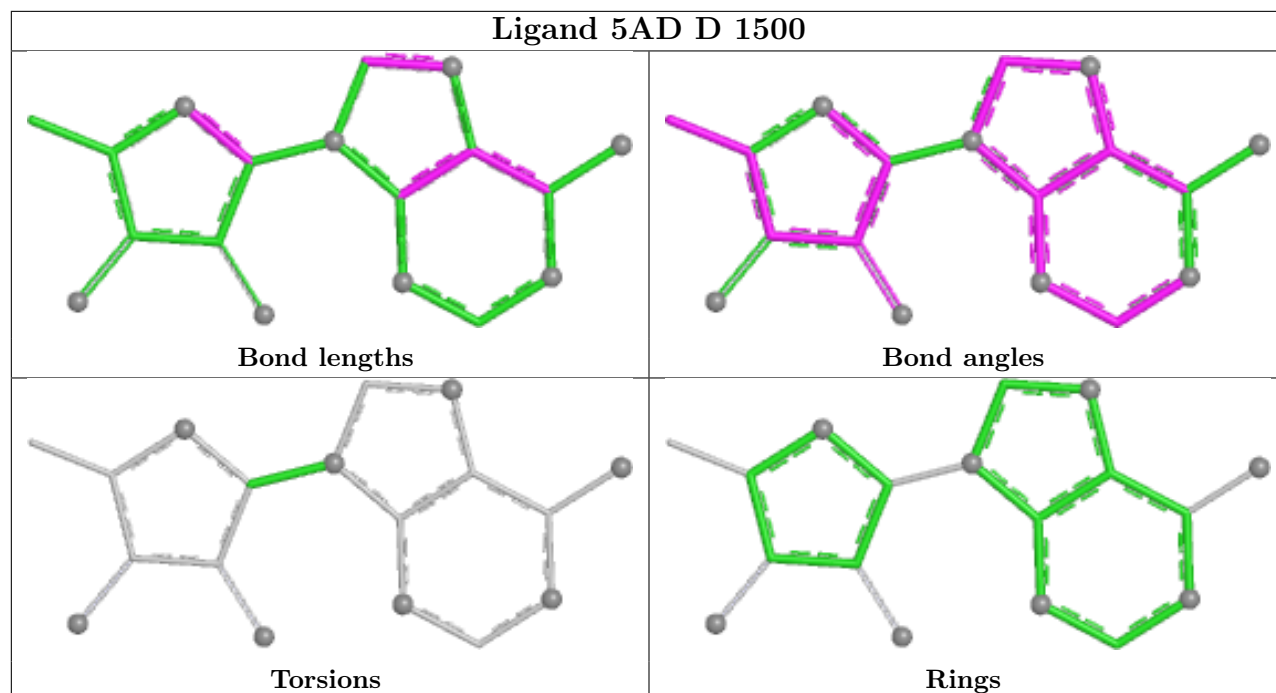
12 monomers are involved in 102 short contacts:

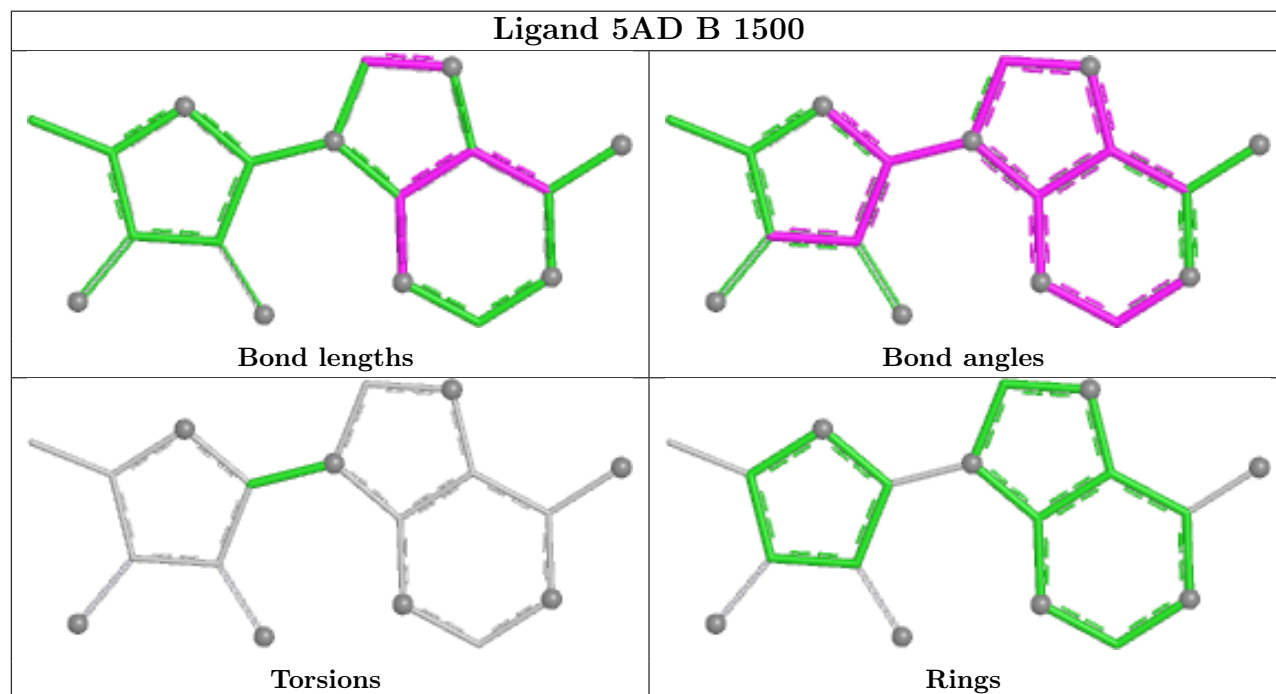
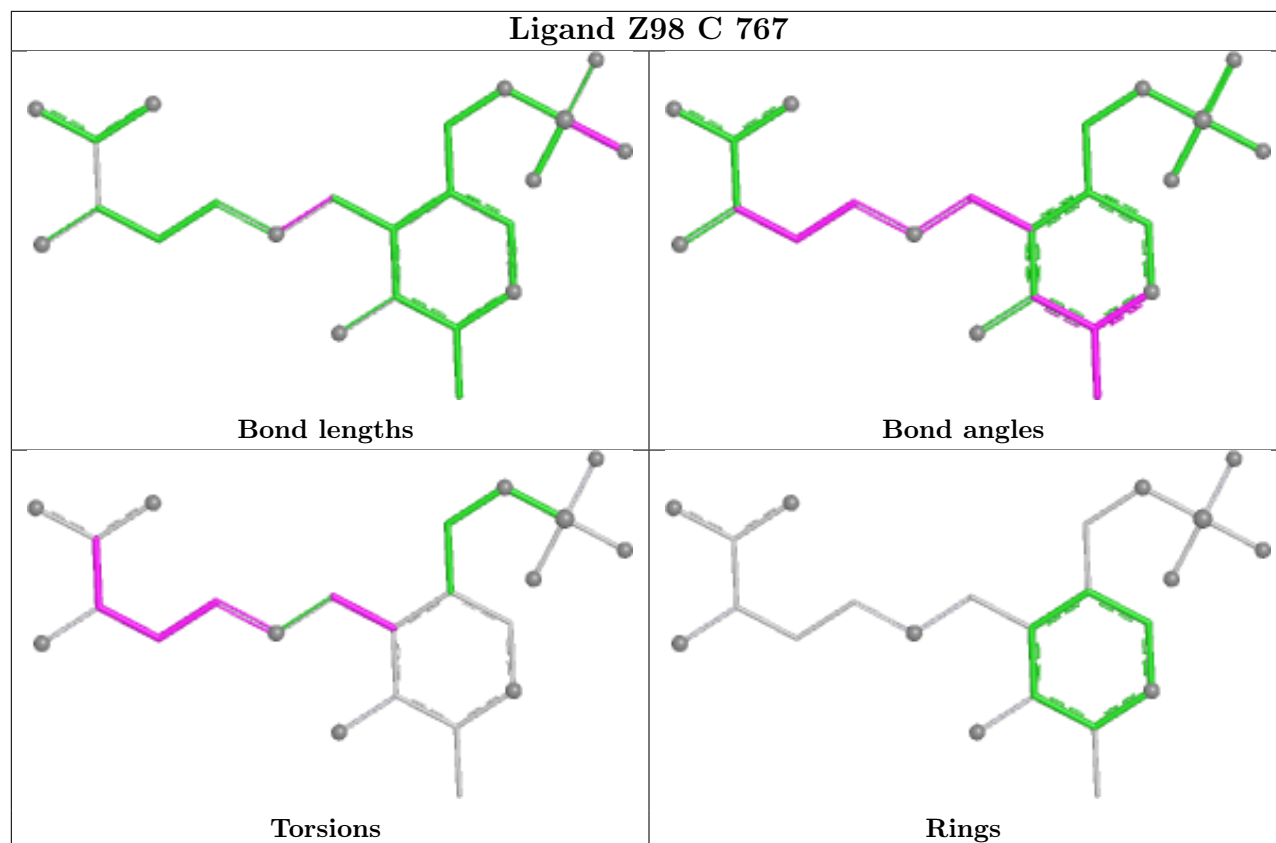
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1500	5AD	3	0
3	A	1801	B12	17	0
3	C	1801	B12	16	0
5	D	767	Z98	8	0
4	D	1500	5AD	4	0
3	D	1801	B12	14	0
5	C	767	Z98	8	0
4	B	1500	5AD	2	0
5	B	767	Z98	8	0
3	B	1801	B12	20	0
4	A	1500	5AD	2	0
5	A	767	Z98	11	0

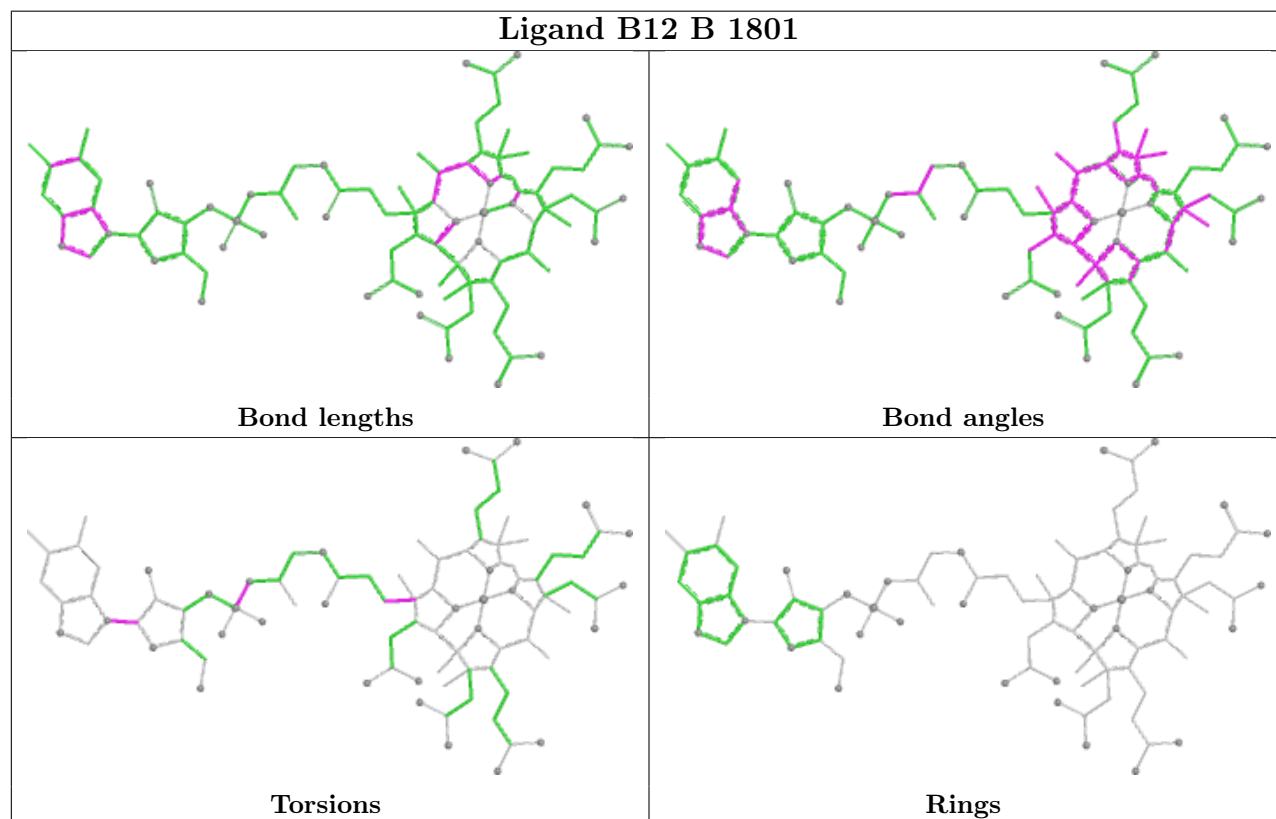
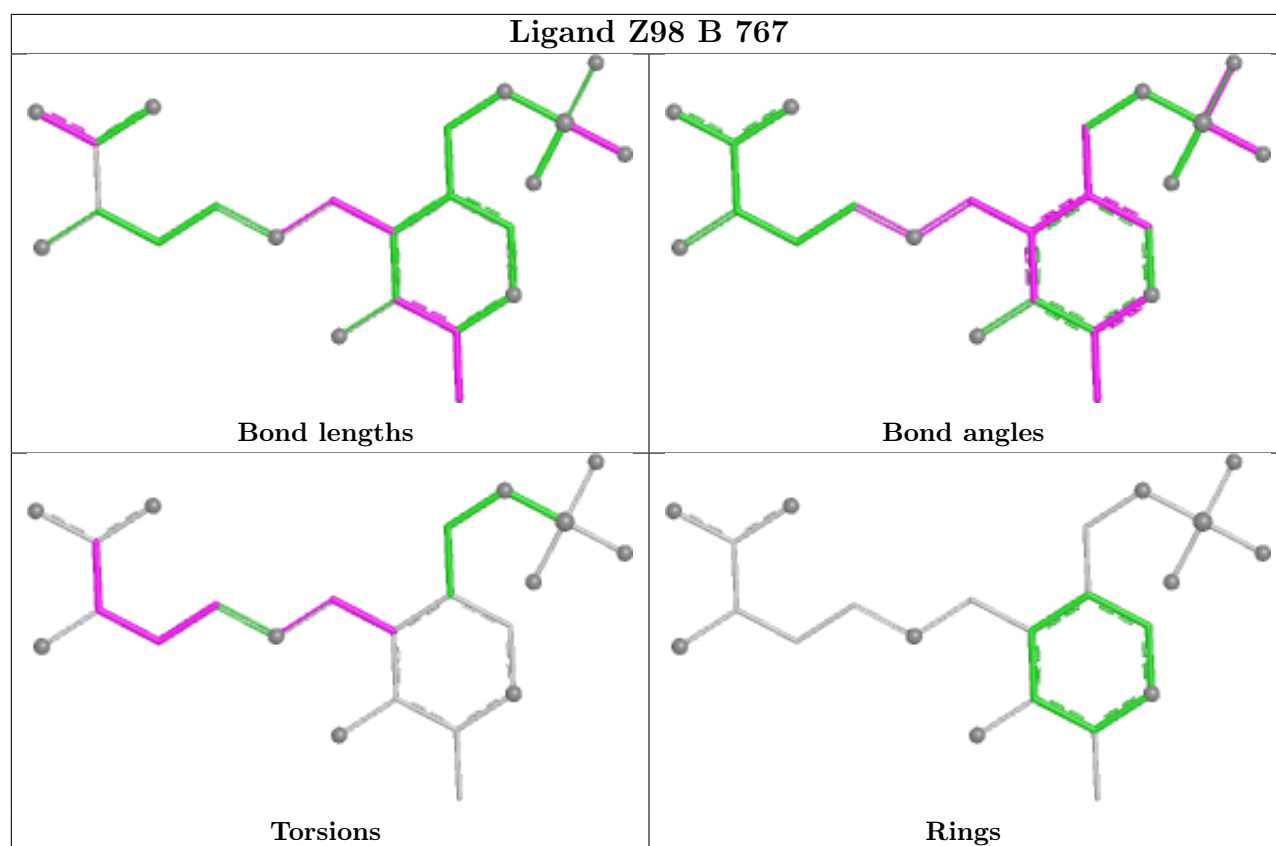
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

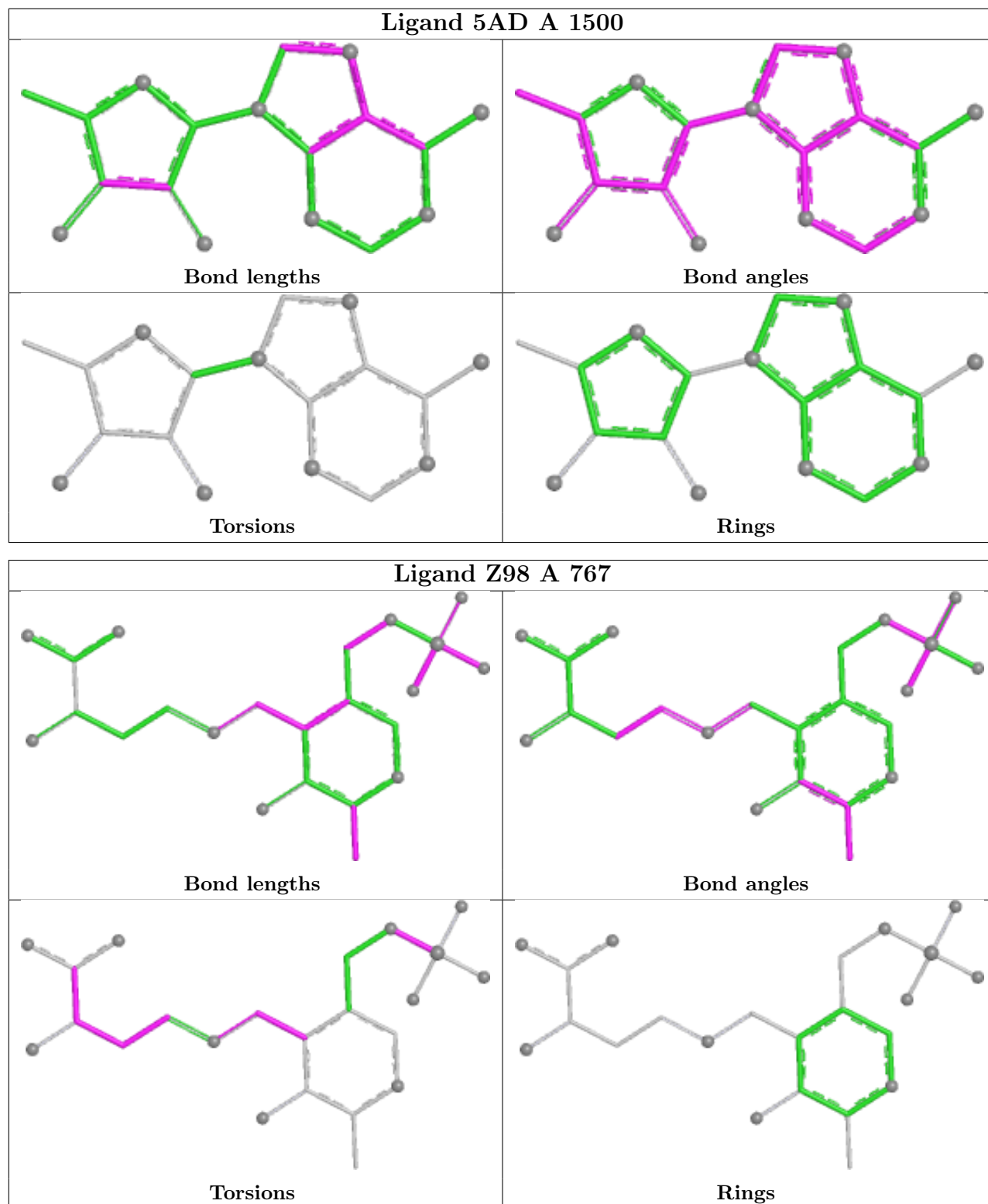












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	728/763 (95%)	-0.11	13 (1%) 67 63	13, 27, 68, 84	0
1	B	728/763 (95%)	-0.46	2 (0%) 90 88	10, 22, 42, 56	0
1	C	728/763 (95%)	-0.30	3 (0%) 88 86	12, 28, 49, 66	0
1	D	728/763 (95%)	-0.37	3 (0%) 88 86	10, 23, 50, 65	0
2	E	109/121 (90%)	-0.17	0 100 100	17, 32, 46, 50	0
2	F	109/121 (90%)	-0.34	1 (0%) 81 78	15, 24, 37, 45	0
2	G	109/121 (90%)	-0.11	0 100 100	24, 35, 50, 55	0
2	H	109/121 (90%)	-0.20	1 (0%) 81 78	15, 27, 45, 61	0
All	All	3348/3536 (94%)	-0.30	23 (0%) 84 81	10, 26, 54, 84	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	ILE	3.9
1	A	683	ILE	3.2
1	B	5	LEU	3.0
1	A	692	ILE	2.7
1	A	688	VAL	2.7
1	C	5	LEU	2.5
1	A	5	LEU	2.5
1	A	709	VAL	2.5
1	C	587	PRO	2.4
1	C	511	ILE	2.4
1	D	6	GLN	2.4
1	A	659	LEU	2.4
1	A	506	ARG	2.3
1	A	587	PRO	2.3
1	A	699	GLY	2.3
1	D	688	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	8	ARG	2.3
1	A	710	ALA	2.2
1	A	686	LEU	2.2
1	D	591	ILE	2.1
2	F	6	ASP	2.1
1	A	657	ILE	2.1
2	H	6	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

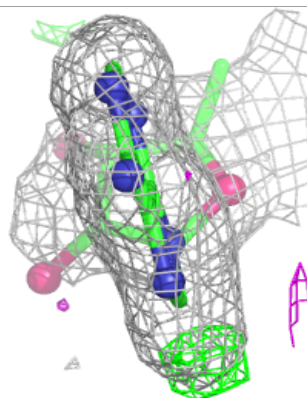
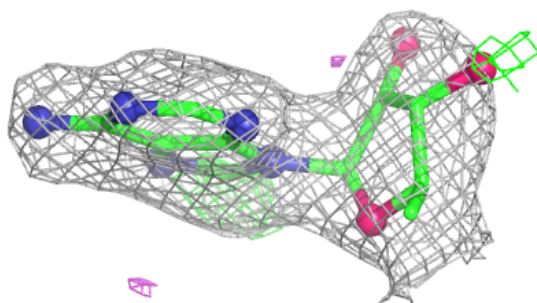
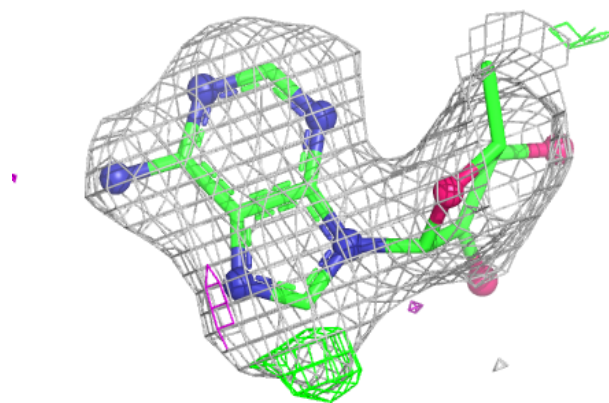
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5AD	C	1500	18/18	0.80	0.13	53,54,55,57	0
4	5AD	D	1500	18/18	0.84	0.13	38,40,45,45	0
4	5AD	A	1500	18/18	0.86	0.13	39,43,47,47	0
4	5AD	B	1500	18/18	0.89	0.09	25,38,42,42	0
3	B12	A	1801	91/91	0.94	0.09	27,43,50,54	0
3	B12	D	1801	91/91	0.95	0.08	19,29,40,43	0
5	Z98	C	767	23/23	0.95	0.09	26,34,43,44	0
5	Z98	B	767	23/23	0.96	0.08	18,23,33,34	0
5	Z98	A	767	23/23	0.96	0.09	21,32,42,43	0
3	B12	B	1801	91/91	0.97	0.06	14,21,29,35	0
3	B12	C	1801	91/91	0.97	0.06	12,23,31,34	0
5	Z98	D	767	23/23	0.97	0.08	19,24,46,46	0

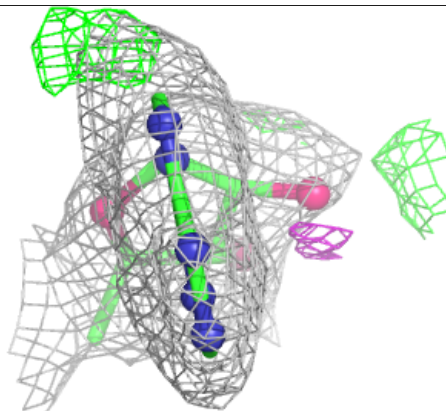
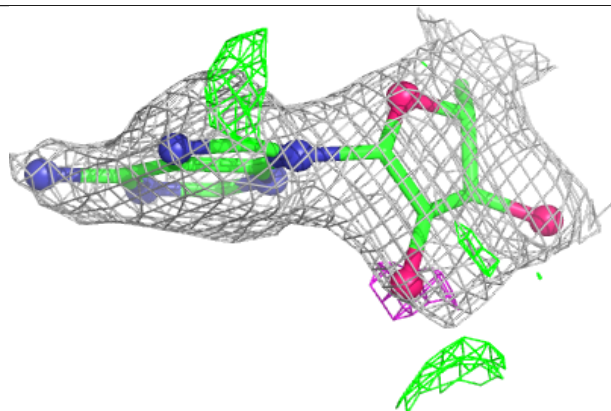
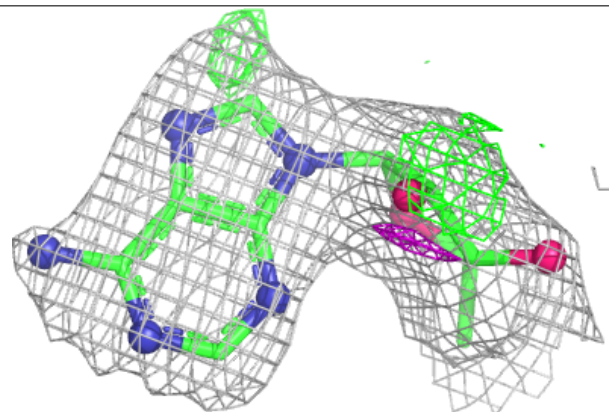
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 5AD C 1500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

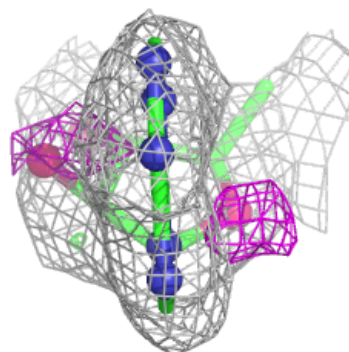
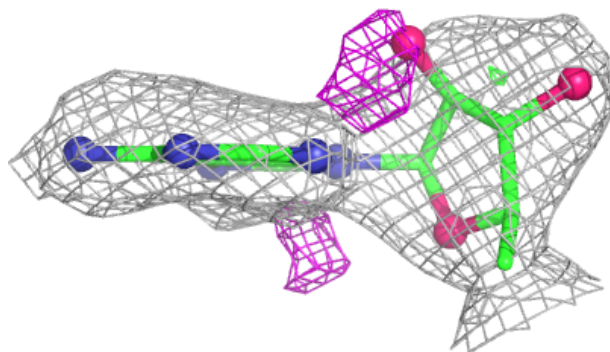
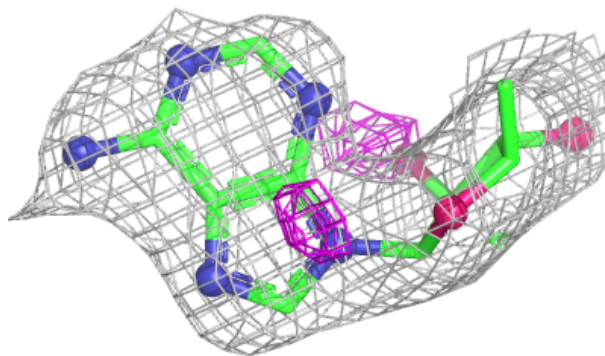
**Electron density around 5AD D 1500:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

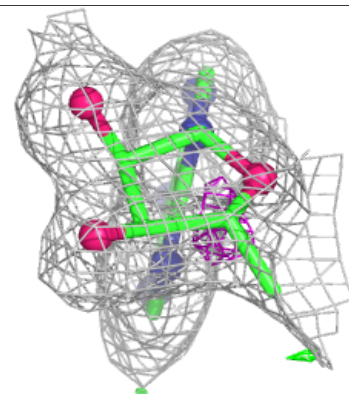
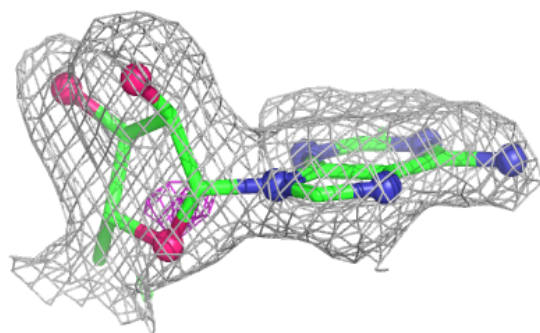
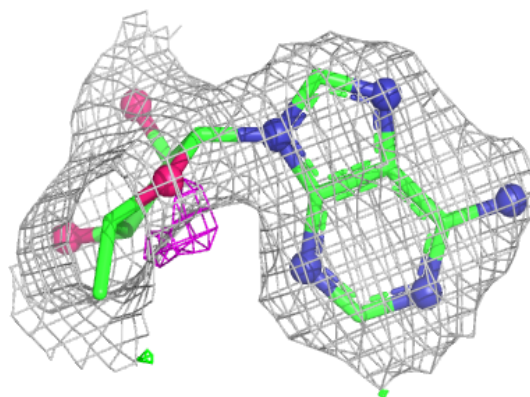


Electron density around 5AD A 1500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

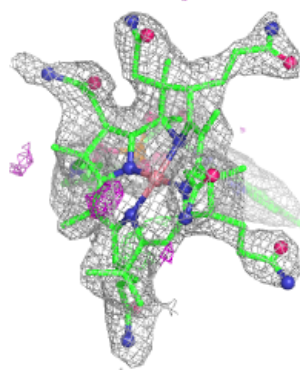
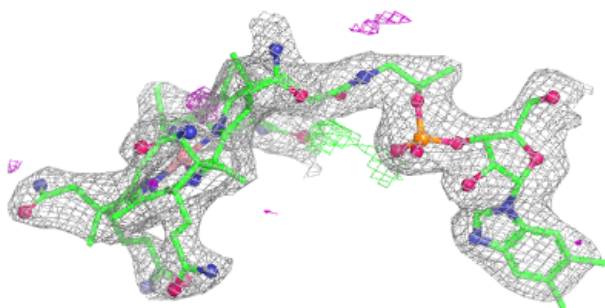
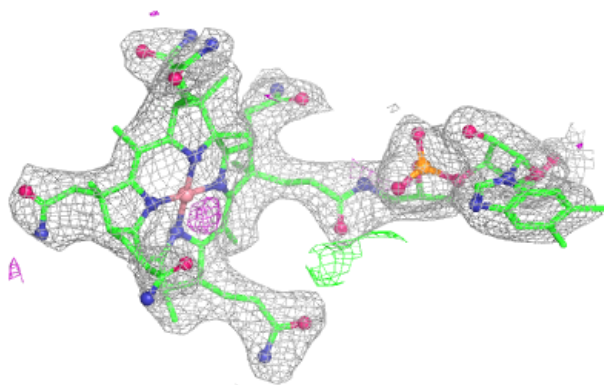
**Electron density around 5AD B 1500:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

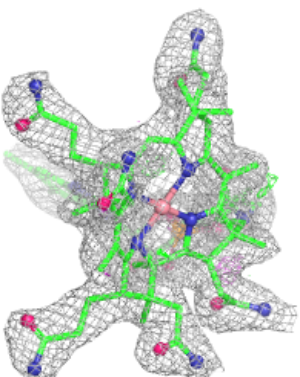
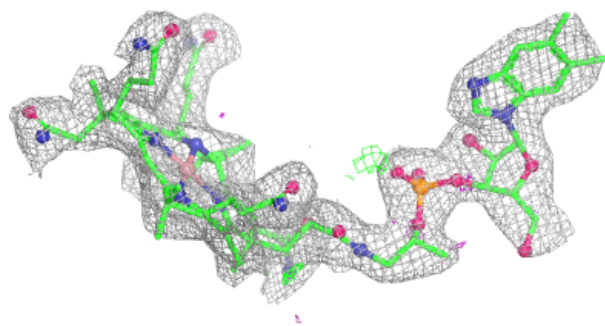
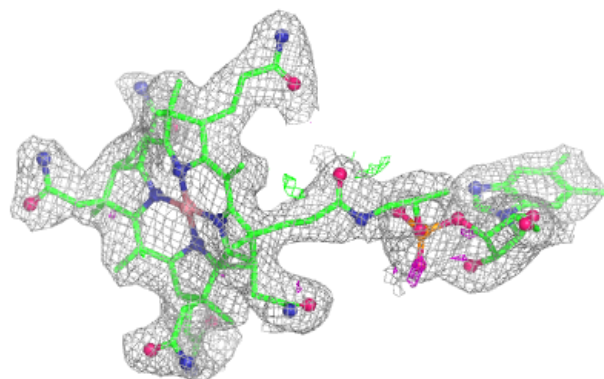


Electron density around B12 A 1801:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

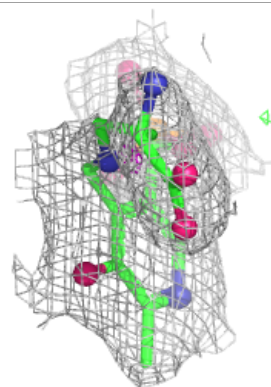
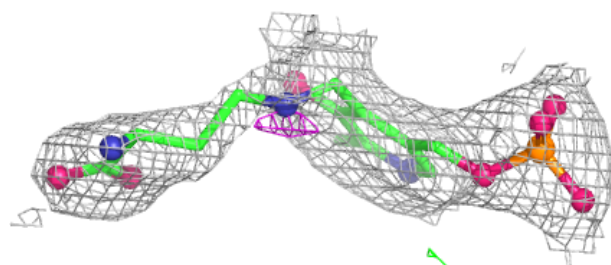
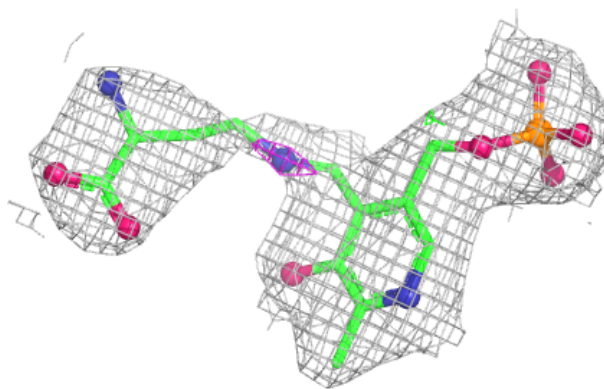
**Electron density around B12 D 1801:**

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and green (positive)

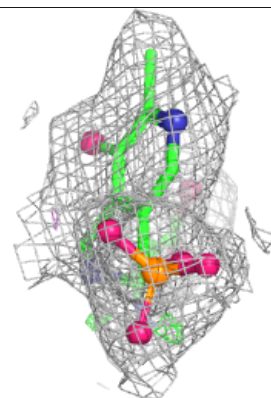
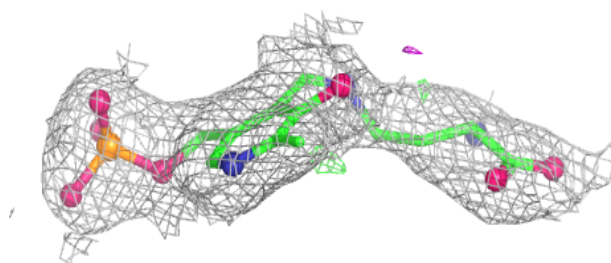
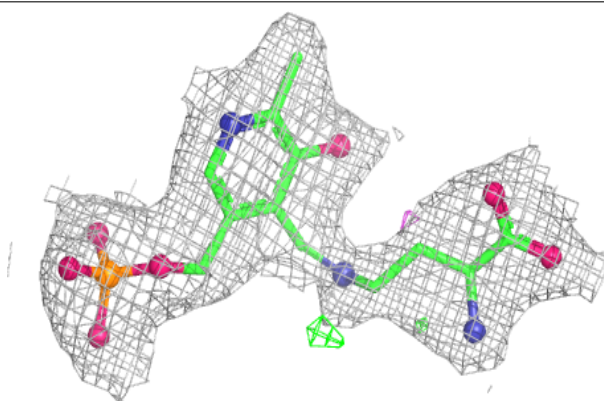


Electron density around Z98 C 767:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

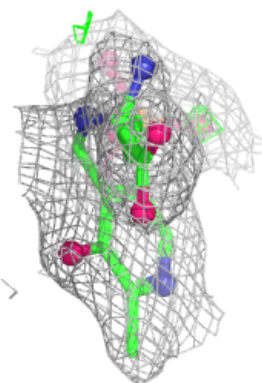
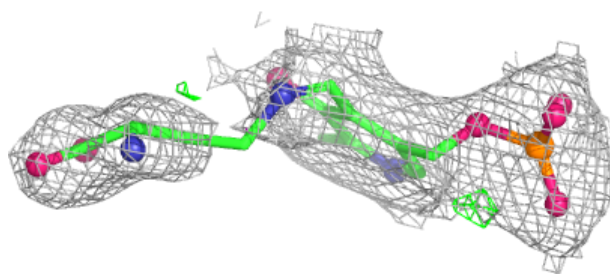
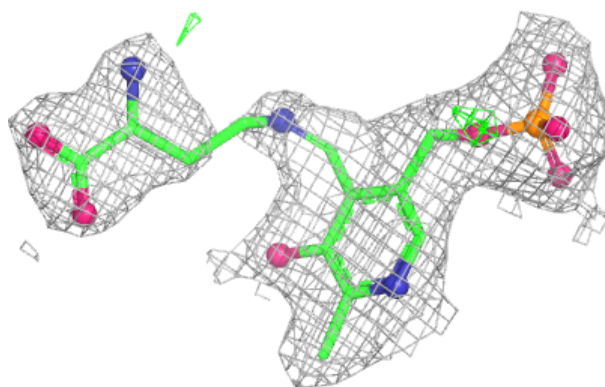
**Electron density around Z98 B 767:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

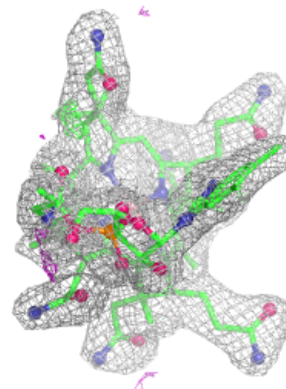
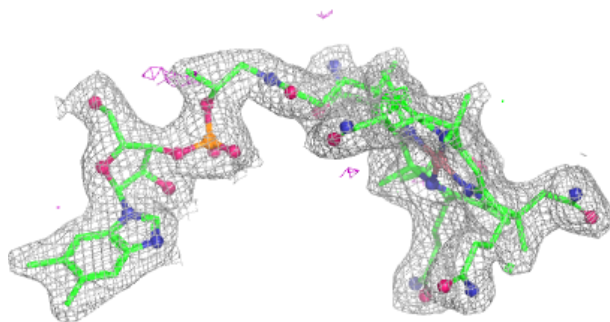
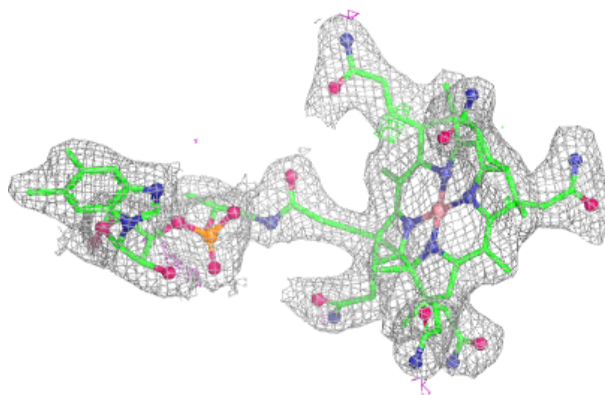


Electron density around Z98 A 767:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

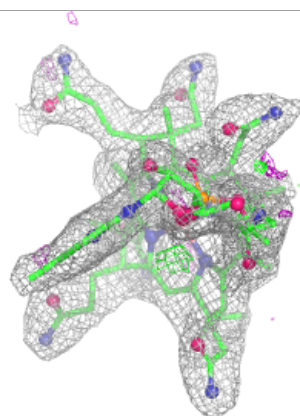
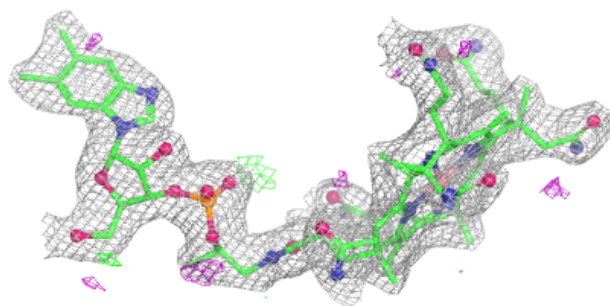
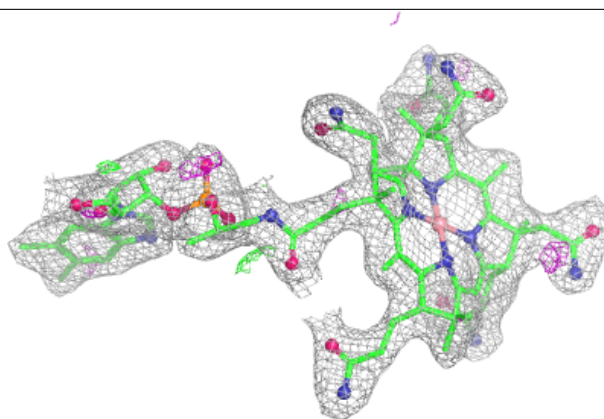
**Electron density around B12 B 1801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

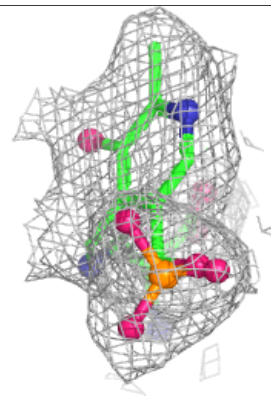
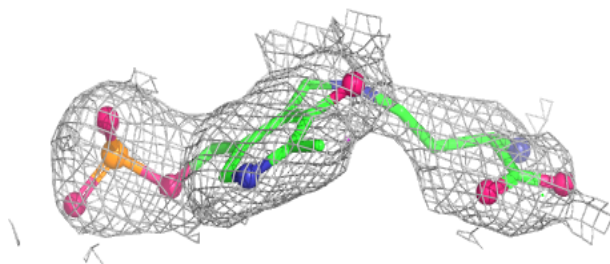
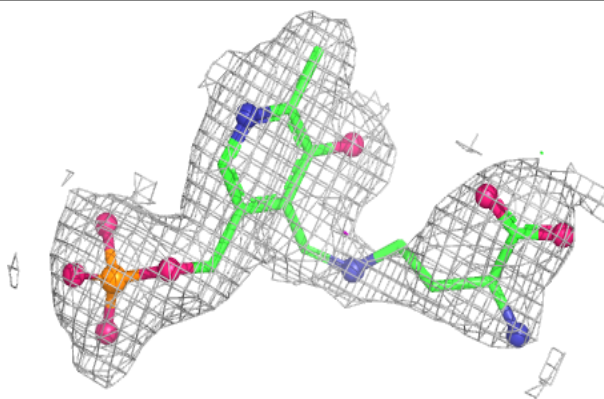


Electron density around B12 C 1801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Z98 D 767:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.